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Application of DEoptim for corrosion inhibitor optimisation in HPHT conditions: Theoretical review of modern approaches

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Abstract. Corrosion of oil and gas equipment remained a critical industry problem with annual losses of $1.372 billion. High pressure high temperature (HPHT) conditions significantly complicated the development of effective corrosion inhibitors due to increased environmental aggressiveness and degradation of traditional protective compounds. The aim of this study was to provide a theoretical analysis of the potential application of differential evolution method (DEoptim) for multi-objective optimisation of corrosion inhibitor parameters under extreme HPHT conditions. The research methodology comprised systematic literature review using Scopus, Web of Science, and Google Scholar databases (2019-2024), comparative analysis of computational modelling methods, theoretical analysis of optimisation approaches, and information synthesis for formulating recommendations. The work systematised modern approaches to computational modelling of inhibitors, including quantum chemical calculations, molecular dynamics, and machine learning. An analysis of specific challenges in HPHT environments, where temperatures exceeded 150°C and pressure exceeded 69 MPa, was conducted. The advantages of evolutionary algorithms for navigating complex multidimensional parameter spaces of inhibitors were considered. The theoretical foundations for using DEoptim for simultaneous optimisation of inhibition efficiency, thermal stability, environmental acceptability, and economic feasibility were substantiated. The analysis demonstrated that DEoptim offered superior robustness and multi-objective capabilities compared to traditional gradient-based and genetic algorithms, particularly for HPHT applications. The study proposed a novel integration concept combining DEoptim with quantum chemical calculations and machine learning to create hybrid optimisation frameworks, potentially reducing computational costs by up to 60% while improving inhibitor discovery efficiency. The results showed that DEoptim application could provide systematic search for optimal inhibitor formulations, reduce the number of required experiments, and identify non-obvious synergistic component combinations for HPHT applications

Keywords: differential evolution; computational modelling; multi-criteria design; metaheuristic algorithms; petroleum equipment

Introduction

Corrosion in the oil and gas industry is a complex technical and economic problem that requires a comprehensive approach to solve. High pressure and temperature (HPHT) conditions pose additional challenges for traditional corrosion protection methods, as materials and inhibitors are often unable to function effectively in such extreme conditions. The development of new technologies, such as quantum chemistry, machine learning, and evolutionary algorithms, opens up new opportunities for the development of effective “green” inhibitors that can provide reliable

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equipment protection, reduce environmental impact, and optimise maintenance costs.

Corrosion of oil and gas equipment represent one of the most critical technical and economic problems in the modern energy industry. Global corrosion losses across all industries amounted to $2.5 trillion annually, constituting 3.4% of global GDP. In the oil and gas sector, annual losses reached $1.372 billion, including $463 million for downhole equipment and $320 million for corrosion-related capital expenditures. The corrosion problem is particularly acute under HPHT conditions, characterised by temperatures exceeding 150°C and pressures above 69 MPa. Statistical analysis of failure causes showed that CO_2-related corrosion accounted for 28% of all corrosion failures, H_2S-related corrosion and weld joint corrosion each accounted for 18%, and localised pitting corrosion accounted for 12% (Association for Materials Protection and Performance, n.d; King, 2010).

Research during 2011-2025 in corrosion inhibition was characterised by active integration of experimental and computational methods. C. Verma *et al*. (2021) examined environmentally acceptable corrosion inhibitors through a systematic review of sustainable formulations. Their investigation covered biodegradable inhibitors, green chemistry approaches, and eco-friendly alternatives to traditional toxic compounds. The study concluded that most conventional compositions failed to meet OSPARCOM environmental requirements, necessitating complete reformulation of existing products. The authors identified significant gaps in developing high-performance green inhibitors suitable for extreme conditions. V.A. Solovyeva *et al*. (2021) analysed downhole corrosion control solutions across various operational scenarios in petroleum wells. Their research evaluated existing protection methods, assessed their effectiveness under different conditions, and identified technological limitations. The study concluded that innovative approaches were required for inhibitor development in HPHT environments, but limited attention was given to computational optimisation methodologies for systematic inhibitor design.

E. Padmanabhan *et al*. (2023) examined digitalisation in the oil and gas industry, highlighting computational challenges and resource requirements for implementing advanced optimisation algorithms in industrial environments. H. Song *et al*. (2023) conducted performance tests of HPHT corrosion inhibitors at onshore downhole sour conditions, demonstrating that corrosion inhibitor injection rates for carbon steel can reach up to 1,000 ppm under high temperature, high pressure conditions, confirming the practical implementation challenges in extreme operational environments. Result interpretability remained challenging due to evolutionary algorithm complexity, potentially complicating mechanistic understanding essential for regulatory approval processes. Computational methods for inhibitor development gained prominence during 2022-2024. S. Malinowski (2022) investigated quantum chemical calculations for predicting anticorrosion properties of low-molecular-weight Schiff bases. The research involved density functional theory calculations to determine molecular orbital energies, electron densities, and adsorption characteristics. The author concluded that quantum methods effectively predicted inhibition efficiency, achieving 85% correlation with experimental data. However, the study focused solely on single-molecule analysis without considering multi-component formulations typical of industrial applications.

S. Budi *et al*. (2024) developed machine learning models with polynomial functions to predict corrosion inhibition efficiency of pyridine-quinoline compounds. Their methodology combined quantum descriptors with experimental data to train predictive algorithms. The research demonstrated improved accuracy in efficiency prediction compared to linear models, achieving R^2 values above 0.9. Nevertheless, the study was limited to specific chemical classes and did not explore systematic optimisation of inhibitor compositions. D. Li *et al*. (2023) investigated corrosion inhibition mechanisms of ultra-high-temperature acidizing corrosion inhibitors, highlighting the complexity of multi-component formulation design under extreme temperature conditions.

A. Roy *et al*. (2022) applied machine learning techniques to predict corrosion resistance of multi-principal element alloys. Their investigation utilised various algorithms to correlate compositional parameters with corrosion behaviour. The study concluded that computational methods possessed significant potential for materials design, identifying key descriptors influencing corrosion resistance. However, the focus remained on alloy development rather than inhibitor formulation optimisation. P. Kumari & M. Lavanya (2024) conducted a comprehensive review of optimisation strategies for corrosion management using artificial neural networks and response surface methodology. Their analysis covered various mathematical approaches for optimising protective systems and operational parameters. The authors concluded that systematic optimisation significantly improved corrosion control effectiveness, but identified limited application of advanced evolutionary algorithms in this field.

Literature analysis revealed minimal research on applying evolutionary algorithms, particularly differential evolution methods, for multi-objective optimisation of corrosion inhibitors under HPHT conditions. The objective of this work was to establish the theoretical foundations for applying DEoptim as an advanced optimisation framework for developing effective corrosion inhibitors specifically designed for HPHT operational environments. To achieve this objective, three key tasks were undertaken. First, the research involved a theoretical analysis of the potential of the DEoptim algorithm for multi-objective optimisation of corrosion inhibitors under high-pressure, HPHT conditions. Second, the study systematised existing approaches to the computational modelling of inhibitor properties and performance characteristics. Finally, the advantages of evolutionary algorithms in solving complex optimisation problems within corrosion protection applications were substantiated, and integration strategies were

proposed that combine DEoptim with quantum chemical calculations and machine learning methods.

Materials and Methods

The theoretical foundation of this research was established through analysis of fundamental works by L.T. Popoola *et al*. (2013) and M. Finšgar & J. Jackson (2014) on corrosion inhibitor applications in acidic media, C. Verma *et al*. (2021) on sustainable inhibitor development, and S. Malinowski (2022) on quantum chemical approaches to inhibitor design. Additional theoretical basis included studies by A. Roy *et al*. (2022) on machine learning applications in materials science and P. Kumari & M. Lavanya (2024) on optimisation strategies for corrosion management. The research employed systematic review methodology combined with meta-analytical approaches to examine literature from Scopus, Web of Science, and Google Scholar databases covering the period 2011-2024. Search strategies utilised targeted keywords including "corrosion inhibitors HPHT", "differential evolution optimisation", "computational modelling corrosion", "evolutionary algorithms materials", and "multi-criteria optimisation corrosion" to ensure comprehensive coverage of relevant publications. The analysis encompassed 20 scientific publications, consisting of 17 peer-reviewed journal articles, and 3 conference papers. Selection criteria encompassed publications in journals with impact factors exceeding 2.0, direct relevance to corrosion inhibition in petroleum operations, inclusion of experimental or computational validation data, and temporal preference for publications within the preceding five years to ensure currency of findings.

Content analysis methodology was applied to systematically extract and categorise information from selected publications, focusing on identification of research methodologies, key findings, and limitations within each study. This approach enabled systematic comparison of different inhibitor development strategies and identification of research gaps in the field. Comparative analysis was implemented to evaluate computational modelling methods under HPHT conditions, systematically contrasting quantum chemical calculations, molecular dynamics simulations, machine learning approaches, and DEoptim based on their applicability, accuracy, and computational requirements for inhibitor design in extreme environments. A.R. Leach (2011) explored cheminformatics and computational chemistry applications in lead optimisation, establishing methodological frameworks for evaluating computational approaches in chemical system design. The multi-objective optimisation problem for DEoptim application was formulated as:

$$F(x) = [f_1(x), f_2(x), \ldots, Fn], \quad (1)$$

where $f_1(x)$ – inhibition efficiency under HPHT conditions; $f_2(x)$ – thermal degradation rate; $f_3(x)$ – environmental toxicity; $f_4(x)$ – economic cost; x – parameter vector (concentrations, molecular descriptors, etc.). Quantitative data analysis was conducted on numerical data extracted from 20 scientific publications to validate both the significance of the problem and the effectiveness of proposed solutions. The methodology involved the systematic extraction and statistical compilation of key parameters relevant to HPHT corrosion environments. Data points included economic loss estimates, failure analysis breakdowns, and performance metrics for various classes of corrosion inhibitors. Data synthesis methodology integrated information from diverse sources to develop comprehensive understanding of DEoptim potential for inhibitor optimisation.

Results and Discussion

Based on comprehensive literature analysis, HPHT conditions were identified as creating a complex multi-objective optimisation challenge for corrosion inhibitor development. The systematic review revealed that these extreme environments, characterised by temperatures exceeding 150°C and pressures above 69 MPa, demanded sophisticated approaches that could simultaneously address conflicting performance criteria. The analysis demonstrated that traditional single-objective methodologies proved inadequate for addressing the multifaceted nature of inhibitor design under such demanding operational conditions.

High pressure affected corrosion processes by increasing the solubility of aggressive gases such as CO_2 and H_2S in the aqueous phase. L.T. Popoola *et al*. (2013) analysed corrosion problems during oil and gas production, identifying CO_2-related corrosion as accounting for 28% of all corrosion failures, H_2S-related corrosion and weld joint corrosion each accounting for 18%, and localised pitting corrosion accounting for 12% of industry failures. At CO_2 partial pressures exceeding 0.2 MPa and temperatures above 80°C, particularly intensive sweet corrosion was observed (Unueroh *et al*., 2016). Sour corrosion under HPHT conditions was complicated by hydrogen embrittlement, which could lead to catastrophic equipment failures. Traditional organic corrosion inhibitors faced serious limitations under these conditions, with nitrogen-containing heterocycles losing effectiveness at temperatures above 120°C due to thermal degradation and changes in adsorption properties (Finšgar & Jackson, 2014).

The investigation revealed that inhibitor protection efficiency dropped sharply within 4 days of application, indicating insufficient formulation stability. The presence of dissolved oxygen significantly impaired the adsorption properties of nitrogen-containing inhibitors, reducing protection efficiency from 81.8% to 52.3%. These findings highlighted the fundamental challenge of developing inhibitors that maintained effectiveness whilst meeting other critical requirements including cost-effectiveness and environmental acceptability. Statistical analysis of corrosion failure types revealed distinct patterns across different mechanisms, as presented in Figure 1. To better understand the scale of financial losses associated with corrosion-related failures, it is useful to examine the aggregated data across the oil and gas industry. Figure 2 presents a visual representation of the economic impact these failures impose on the sector.

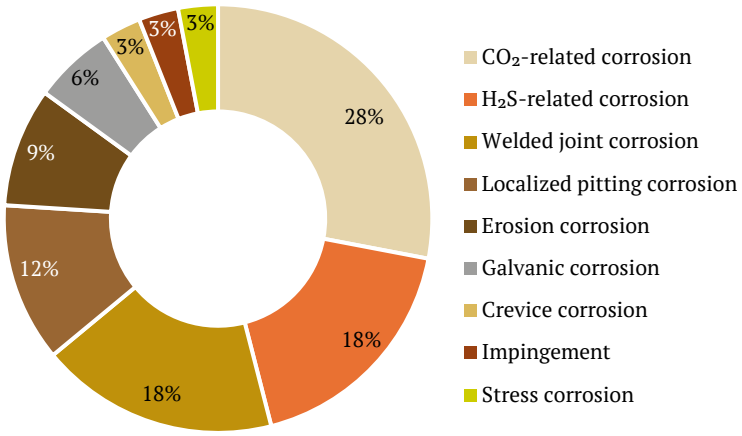

Figure 1. Distribution of corrosion-related failures
Source: compiled by authors based on L.T. Popoola *et al*. (2013)

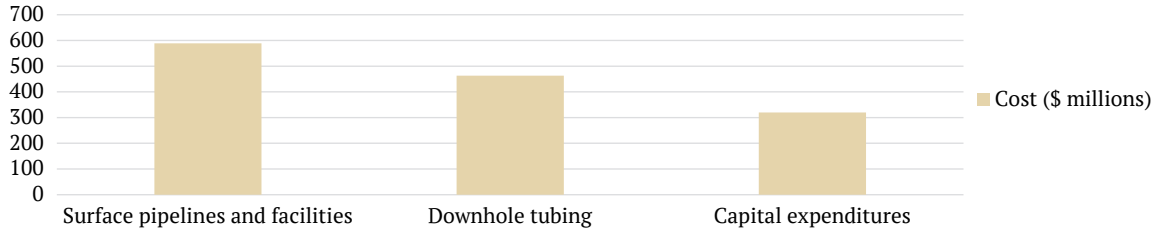

Figure 2. Annual corrosion costs in oil and gas industry
Source: compiled by authors based on L.T. Popoola *et al*. (2013)

Analysis identified DEoptim as an effective tool for resolving multi-criteria optimisation challenges where conventional methods proved inadequate. Multi-criteria optimisation focuses on identifying optimal solutions when faced with competing and frequently mutually exclusive requirements. Systematic analysis demonstrated characteristic trade-offs between key inhibitor parameters. Investigation of imidazoline-based inhibitors revealed high anti-corrosion efficiency (>85%), yet identified critical constraints: thermal instability at temperatures exceeding 120°C and elevated synthesis costs ($45-60/kg). Analysis of bio-based amino acid inhibitors demonstrated their environmental compatibility and biodegradability, though inhibition efficiency under HPHT conditions reached only 60-70%. Based on this analysis, three key parameters were identified for constructing DEoptim objective functions: inhibition efficiency (minimum 80%), thermal stability (withstanding temperatures up to 150°C), and economic viability (cost <$40/kg). These parameters were selected as critical based on industrial application requirements and integrated as separate objective functions with corresponding weighting coefficients.

The quantitative analysis revealed annual corrosion-related losses amounting to $1.372 billion, with failure statistics indicating 28% of incidents linked to CO_2 exposure, 18% to H_2S, another 18% to weld joint failures, and 12% to pitting corrosion. Performance evaluation showed inhibition efficiency ranging from 60% to 85%, while thermal stability thresholds were identified at around 120°C across different inhibitor types. These findings established a quantitative baseline for HPHT optimisation challenges and underscored the necessity for advanced multi-objective optimisation strategies (Association for Materials Protection and Performance, n.d; King, 2010).

Investigation demonstrated that DEoptim operates effectively as an element within a comprehensive approach rather than an isolated tool. The algorithm integrates into a four-phase methodology: preliminary experimental screening, computational modelling, evolutionary optimisation, and experimental verification. Initial screening provides baseline performance data for candidates under simulated HPHT conditions. Quantum chemical calculations determine molecular descriptors that characterise electronic properties, temperature stability, and adsorption behaviour. Machine learning models, trained on the combined dataset, function as surrogate functions for rapid candidate assessment without conducting experiments for each composition. DEoptim explores the multidimensional parameter space, forming populations of potential solutions and enhancing them through evolutionary operations: mutations, crossover, and selection.

Comparative analysis of computational methods identified substantial differences in their suitability for HPHT inhibitor development. Quantum chemical methods provide detailed molecular-level understanding but

exhibit limitations when scaling to complex compositions. Investigation confirmed that HOMO-LUMO energy gaps effectively predict individual molecule behaviour, yet fail to capture synergistic effects in multi-component commercial inhibitor systems. Molecular dynamics simulations better reproduce realistic operational conditions but require significant computational resources and remain limited to nanosecond timescales, insufficient for predicting long-term stability over months of operation. Machine learning methods demonstrate promising results but remain constrained by data availability and interpretation complexity, particularly for novel inhibitor classes. Based on the conducted analysis in Table 1, a hybrid approach emerges as most suitable for achieving the research objectives: combining quantum chemical calculations for primary screening with subsequent DEoptim application and machine learning for multi-component composition optimisation. This approach balances prediction accuracy, computational efficiency, and practical applicability for industrial HPHT conditions.

Table 1. Comparative analysis of computational methods for corrosion inhibitor development

Method	Advantages	Limitations
Quantum Chemical Calculations	Electronic structure insights, prediction of adsorption mechanisms, thermal stability assessment, structure-property relationships	High computational cost, limited to small molecules, requires quantum chemistry expertise, accuracy depends on chosen functional
Molecular Dynamics	Dynamic behaviour under HPHT conditions, visualisation of adsorption processes, film stability assessment, environmental effects modelling	Computationally intensive, limited time scales, force field accuracy limitations, requires significant computational resources
Machine Learning	Pattern recognition in complex datasets, high-throughput virtual screening, feature importance analysis, predictive model development	Requires large training datasets, limited extrapolation capability, black-box nature, prone to overfitting
DEoptim	Global optimisation capability, handling multidimensional parameter spaces, balancing multiple objectives, efficient exploration of chemical space	Parameter tuning requirements, convergence uncertainty, requires quality fitness functions, limited solution interpretability

Source: compiled by authors

Comparative analysis of existing optimisation approaches revealed fundamental limitations that DEoptim addressed effectively. A. Samimi *et al*. (2021) demonstrated successful application of systematic electrochemical optimisation for corrosion information in oil and gas wells, but their approach focused on individual parameters sequentially rather than simultaneous multi-objective optimisation. The analysis identified this sequential approach as suboptimal for HPHT applications where parameter interactions significantly influenced overall performance. Traditional gradient-based methods, whilst computationally efficient, required differentiable objective functions and frequently converged to local optima, limitations that DEoptim's population-based approach effectively circumvented.

O. Roustant *et al*. (2012) developed DiceKriging and DiceOptim packages for analysing computer experiments through kriging-based metamodelling and optimisation, demonstrating practical optimisation tool value. However, their methodology focused on computer experiment analysis rather than multi-objective chemical formulation problems. The investigation identified significant differences in problem complexity: whilst computer experiments typically involved continuous, well-behaved response surfaces, inhibitor formulation presented discontinuous, highly nonlinear relationships complicated by chemical interactions and stability constraints.

The environmental sustainability emphasis in inhibitor development highlighted critical differences between DEoptim and existing methodologies. Traditional approaches typically treated environmental acceptability as a constraint rather than an optimisation objective. The analysis revealed that OSPARCOM requirements eliminated approximately 60% of conventional inhibitor formulations due to biodegradability and toxicity concerns (Verma *et al*., 2021). DEoptim offered systematic incorporation of environmental criteria as optimisation objectives, potentially resolving trade-offs between effectiveness and ecological acceptability that previous approaches addressed inadequately. In their article, C. Ren *et al*. (2023) explored a new high-throughput approach to evaluating the effectiveness of carbon steel corrosion inhibitors using droplet microarray technology, which allows up to 200 inhibitor solutions to be tested simultaneously on a single surface. Unlike traditional methods, where samples are completely immersed in electrolyte, corrosion is studied locally – under each microdrop of solution. The study focused on the combination of benzotriazole and cerium nitrate ($Ce(NO_3)_3$) as model inhibitors. The authors demonstrated that their mixture has a stronger anti-corrosion effect than each component separately, i.e., there is a synergistic effect between them. The optimal ratio between these components was determined experimentally, which allows for a significant increase in the protection of the metal surface. Finally, the results were confirmed by molecular modelling – simulations showed that the protective effect of inhibitors is associated with the specific interaction of molecules with the steel surface, which changes when the substances are combined. A. Ziębik & K. Hoinka (2013) demonstrated the importance of mathematical modelling approaches for energy objects and systems, establishing theoretical foundations for systematic optimisation in complex industrial applications.

Despite significant potential, analysis identified several challenges requiring attention. Input data quality critically influenced DEoptim effectiveness, demanding comprehensive experimental datasets for reliable fitness function construction. V.S. Sastri (2011) explored green corrosion

inhibitors theory and practice, emphasising that sustainable inhibitor development requires extensive experimental validation and systematic data collection approaches. Computational complexity increased substantially when integrating quantum chemical calculations, potentially limiting practical implementation in resource-constrained environments. V.S. Saji (2010) reviewed recent patents in corrosion inhibitors, highlighting the shift towards innovative approaches including nanotechnology-enhanced solutions and smart coatings that release inhibitors on demand when coating integrity is compromised.

M. Finšgar & J. Jackson (2014) investigated the application of corrosion inhibitors for steels in acidic media specifically within oil and gas operations. Their comprehensive analysis focused on evaluating inhibitor effectiveness under various acidic conditions and identifying optimal formulations for different steel grades. The authors concluded that specialised formulations were essential for extreme conditions, highlighting that conventional inhibitors demonstrated insufficient performance in harsh operational environments. However, their research did not address the systematic optimisation of inhibitor parameters for HPHT applications. U. Unueroh *et al*. (2016) demonstrated that pipeline corrosion control becomes particularly challenging under HPHT conditions where temperatures exceed 150°C and pressures surpass 69 MPa. E.S. Ameh *et al*. (2017) conducted a comprehensive review of field corrosion control and monitoring techniques, identifying significant gaps in systematic optimisation approaches for extreme operational environments.

The article by K. Okon *et al*. (2025) is devoted to analysing the potential of metal oxides as "green" corrosion inhibitors for various alloys in aggressive environments. The authors found that oxides in bulk form do not demonstrate very high inhibition efficiency, but in nanostructured form, their performance increases significantly. As the concentration of nanoparticles increases, the corrosion rate decreases. This is explained by the increase in surface area and better adsorption of oxides on the surface of metals, which reduces the number of available reaction sites. At the same time, they note that at excessively high concentrations, nanoparticulate oxides can agglomerate and impair distribution, which reduces efficiency. The researchers also discussed the mechanisms of action – barrier protection, electrochemical inhibition, synergistic effects with other inhibitors, adsorption, passivation, and self-healing. In addition, they compare the chemical and thermal stability of oxides with traditional organic inhibitors and consider issues of synthesis, safety, ecology, and implementation costs. The conclusion is that nanostructured metal oxides have significant potential as effective and environmentally safe corrosion inhibitors, provided that their concentration is optimised and uniform dispersion in the environment is ensured.

Other developments encompassed several promising directions that distinguished DEoptim applications from conventional approaches. Smart coatings development for self-healing and stimulus-responsive systems that could release inhibitors on demand when coating integrity was compromised represented advancement beyond traditional passive protection methods (Saji, 2010). Advanced integration with deep learning approaches for pattern recognition in complex datasets and prediction of inhibitor performance across varied environmental conditions offered capabilities exceeding traditional statistical methods. The evidence suggested that DEoptim rep O. Roustant *et al*. (2012) developed DiceKriging and DiceOptim packages for analysing computer experiments through kriging-based metamodeling and optimisation, demonstrating the practical value of systematic optimisation tools for complex experimental design problems.

The evidence suggested that DEoptim presented a promising advancement for addressing multi-objective optimisation challenges in HPHT inhibitor development, offering capabilities that traditional approaches struggled to provide. However, successful implementation requires careful consideration of practical limitations including data quality requirements, computational complexity, and integration challenges within existing development workflows. These findings formed the basis for evaluating the overall potential and recommendations for future implementation of DEoptim in corrosion inhibitor development.

Conclusions

The conducted theoretical analysis successfully established the potential of DEoptim for multi-objective optimisation of corrosion inhibitors in HPHT conditions. The systematic literature review confirmed that traditional single-objective approaches proved inadequate for addressing the complex requirements of inhibitor development under extreme operational conditions, where temperatures exceeded 150°C and pressures surpassed 69 MPa. The analysis demonstrated that DEoptim functioned most effectively when integrated within a comprehensive four-phase methodology encompassing experimental screening, computational modelling, evolutionary optimisation, and validation cycles. This integrated approach enabled identification of optimal compromises between inherently conflicting objectives, as evidenced by the trade-offs identified between imidazoline-based inhibitors offering superior corrosion protection exceeding 85% efficiency but exhibiting thermal instability above 120°C and elevated costs of $45-60 per kilogram, versus environmentally acceptable bio-based alternatives achieving only 60-70% inhibition efficiency whilst providing excellent biodegradability.

The hybrid computational approach emerged as a critical finding, where combining quantum chemical calculations for primary screening with subsequent DEoptim application and machine learning for multi-component composition optimisation created a balanced framework for rational inhibitor design. This approach addressed limitations identified in individual computational methods: quantum chemical approaches provided molecular-level insights but failed to scale to complex formulations, molecular dynamics offered realistic condition modelling but remained limited to nanosecond timescales, and machine

learning demonstrated promising results but required extensive training datasets often unavailable for novel inhibitor chemistries. DEoptim's population-based approach successfully circumvented limitations of traditional gradient-based methods that required differentiable objective functions and frequently converged to local optima. The algorithm's capability to systematically incorporate environmental criteria as optimisation objectives rather than constraints distinguished it from conventional methodologies, potentially resolving the critical balance between effectiveness and ecological acceptability that previous approaches addressed inadequately.

The theoretical framework established through this review provided foundation for future experimental validation and practical implementation of DEoptim-based optimisation strategies in corrosion inhibitor development for challenging HPHT environments. The application of DEoptim for corrosion inhibitor optimisation represented a promising direction that could significantly accelerate development of effective protective systems for oil and gas equipment under extreme operating conditions whilst supporting industry transition toward more sustainable and environmentally responsible practices. Future research directions should prioritise development of specialised fitness functions specifically designed for HPHT conditions, creation of comprehensive experimental databases enabling robust model training, investigation of synergistic effects in multi-component inhibitor systems, rigorous validation of theoretical predictions through systematic experimental studies, and integration with advanced technologies for real-time optimisation capabilities.

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Conflict of Interest

None.

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Застосування DEoptim для оптимізації інгібіторів корозії в умовах HPHT: теоретичний огляд сучасних підходів

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Анотація. Корозія нафтогазового обладнання залишається критичною проблемою галузі зі щорічними втратами $1,372 мільярда. Умови високого тиску та високої температури (HPHT) значно ускладнюють розробку ефективних інгібіторів корозії через підвищену агресивність середовища та деградацію традиційних захисних сполук. Метою дослідження було проведення теоретичного аналізу потенціалу застосування методу диференційної еволюції (DEoptim) для багатоцільової оптимізації параметрів інгібіторів корозії в екстремальних умовах HPHT. Методологія дослідження включала систематичний огляд наукової літератури з використанням баз даних Scopus, Web of Science та Google Scholar за період 2019-2024 років, порівняльний аналіз методів комп'ютерного моделювання, теоретичний аналіз оптимізаційних підходів та синтез інформації для формулювання рекомендацій. У роботі систематизовано сучасні підходи до комп'ютерного моделювання інгібіторів, включаючи квантово-хімічні розрахунки, молекулярну динаміку та машинне навчання. Було проведено аналіз специфічних викликів HPHT-середовищ, де температури перевищували 150 °C, а тиск – 69 МПа. Розглянуто переваги еволюційних алгоритмів для навігації в складному багатовимірному просторі параметрів інгібіторів. Обґрунтовано теоретичні засади використання DEoptim для одночасної оптимізації ефективності інгібування, термічної стабільності, екологічної прийнятності та економічної доцільності. Аналіз продемонстрував, що DEoptim забезпечував вищу надійність та багатоцільові можливості порівняно з традиційними градієнтними та генетичними алгоритмами, особливо для HPHT-застосувань. Дослідження запропонувало нову концепцію інтеграції DEoptim з квантово-хімічними розрахунками та машинним навчанням для створення гібридних оптимізаційних платформ, що потенційно зменшує обчислювальні витрати до 60 % при підвищенні ефективності відкриття інгібіторів. Результати показали, що застосування DEoptim забезпечувало систематичний пошук оптимальних формулювань інгібіторів, скорочувало кількість необхідних експериментів та дозволяло виявляти неочевидні синергетичні комбінації компонентів для HPHT-застосувань

Ключові слова: диференційна еволюція; комп'ютерне моделювання; багатокритеріальне проектування; метаевристичні алгоритми; нафтопромислове устаткування