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Metaheuristic Methods for Chemical Reactor Design and Process Optimization A Methodological Perspective

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Abstract

Chemical reactor and process optimization combines nonlinear models, constraints, mixed design variables and competing engineering objectives. This methodological perspective examines how evolutionary and swarm search can be represented, constrained and evaluated in that setting. It distinguishes algorithm descriptions from evidence of performance, surrogate accuracy from physical validation, and offline design from safety-critical online control. The documentary scope is narrative rather than a verified systematic corpus: the reported screening counts are unreconciled, and the retained generic plots do not establish reactor-specific experimental results. The analysis emphasizes feasibility, matched evaluation budgets, reproducible simulation models, suitable statistical units and explicit trade-offs among production, energy, environmental and safety objectives. It provides criteria for future reactor optimization studies without asserting an optimizer ranking or a complete synthesis of 179 chemical engineering papers.

Keywords: Metaheuristic optimization, Chemical reactor design, Process optimization, Constraint handling, Multi-objective optimization, Reproducibility.

1 | Introduction

Chemical reactor design and operation require selecting variables such as geometry, residence time, feed composition and temperature under a physical model and operating constraints. Nonlinearity and expensive simulation can make stochastic search useful, but a candidate with a good objective value is not automatically

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physically feasible or safe. This perspective examines the methodological connection between a search procedure, a reactor model and the evidence needed to support an engineering decision.

The algorithm families considered include genetic search [1], particle swarm optimization [2], differential evolution [3], artificial bee colony search [4], grey wolf optimization [5], whale optimization [6], Harris hawks optimization [7] and covariance-matrix adaptation [8]. Their update mechanisms are general computational tools. The quality of a reactor study depends additionally on its representation, simulator, constraints, parameter estimates and validation protocol.

There is no universal ranking of these methods established by the present narrative. A finite benchmark result supports the tested settings and problem instances. It does not demonstrate that one algorithm dominates every reactor model, budget or constraint regime, and an absence of a universal winner does not logically require inventing more biological metaphors.

A methodological synthesis can help separate algorithm identity from engineering evidence. In reactor design, the issues of variable representation, model uncertainty, nonlinear feasibility and competing objectives are central. Domain-specific review literature explicitly treats reactor production objectives and evolutionary multi-objective approaches [9]. The present perspective uses that scope to organize evaluation requirements, rather than to estimate publication frequencies.

The analysis proceeds from problem structure to optimizer representation, then to evidence, validity limits and future research. Its contribution is a critical set of evaluation criteria. It does not claim a reproducible bibliometric census, a pooled optimizer performance analysis or exhaustive coverage of all chemical process applications.

Cross-domain algorithm reuse is useful when the mathematical role of each component is made explicit. A chemical metaphor used to name an optimizer does not supply a kinetic model, mass balance or thermodynamic constraint. Conversely, an algorithm inspired by another domain can be relevant if it can handle the reactor formulation and its evaluation cost.

2 | Background and Context

The background separates the objective and feasible set supplied by chemical engineering from the numerical rules used to search them. These are distinct sources of assumptions and uncertainty.

2.1 | Definitions and Fundamental Concepts

A metaheuristic is a search framework that guides candidate generation and evaluation without generally certifying a global optimum. It may use one trajectory or a population, and its randomization and acceptance rules must be specified. Exploration and exploitation describe search behavior, not intrinsic quality labels. Their usefulness depends on representation, budget and objective landscape.

In reactor optimization the search state must preserve the meaning and units of design variables. Continuous temperatures or feed rates, integer unit counts and discrete equipment choices require different encodings. Fitness must correspond to a defined physical or economic objective, while constraints must describe mass and energy balances, bounds and operating feasibility. A penalty value alone does not certify satisfaction of these constraints.

2.2 | Historical Evolution

Genetic search combines selection with variation [1], PSO uses personal and shared best positions [2], and DE forms candidates from population differences [3]. Later families use distinct update schedules and selection mechanisms [5–7]. CMA-ES adapts a Gaussian search covariance and step size [8]. Chronological novelty does not establish a superior reactor optimizer.

Landscape and sensitivity analyses can reveal whether changes in a variable materially affect a model output. They require a specified simulator, input domain and sampling design. A plotted effect score cannot establish reactor sensitivity without those ingredients, and neither low-dimensional benchmark behavior nor a response-surface visualization supplies a chemical validation argument.

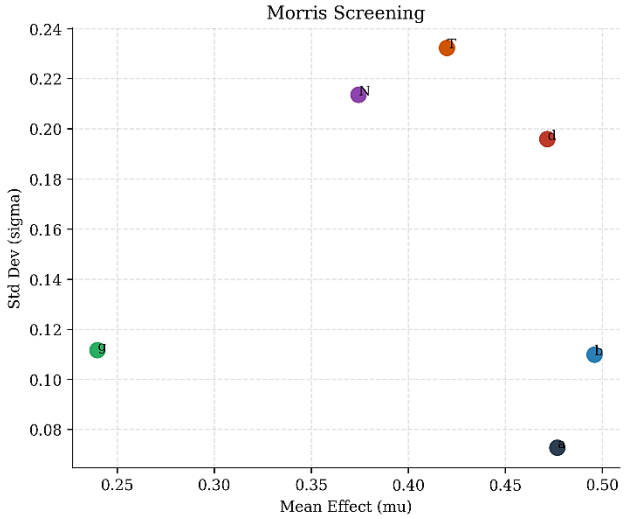


Fig.1. Retained elementary-effects screening illustration.

The simulator, factor ranges and evaluation logs are not specified, so the plot is not reactor-specific sensitivity evidence (*Fig. 1*).

3 | Review Methodology

The review record states that IEEE Xplore, ScienceDirect, SpringerLink, Wiley, ACM Digital Library and Google Scholar were considered over 2000-2025, with algorithm, application, peer-review and language criteria. However, exact search dates and strings, deduplication rules, eligibility decisions and a complete included-study register are not documented. *Table 1* preserves the reported counts. Its final-selection total is 554, whereas the documentary inclusion claim is 179 papers. These numbers cannot be interpreted as a verified screening flow without the original records.

Table 1. Reported database counts awaiting screening-flow reconciliation.

Database	Results	Final Selection
IEEE xplore	850	180
Sciencedirect	620	130
Springer link	450	95
Wiley online	280	60
ACM digital library	180	35
Google scholar	120	25
Total	2,500	554

Note: Entries are retained documentary counts, not a verified systematic-review corpus.

A systematic synthesis would require a traceable row for every included reactor study, connecting its citation to reactor type, physical model, objectives, constraints, optimizer configuration, baseline budget and validation evidence. The present bibliographic record does not establish such a 179-paper register or a 554-paper final selection. Consequently, frequencies, trends and aggregate optimizer rankings are not estimated here.

4 | Survey of Metaheuristic Algorithms

The following algorithm discussion focuses on representation and evaluation requirements. It does not rank their reactor performance from the qualitative labels in *Table 2*.

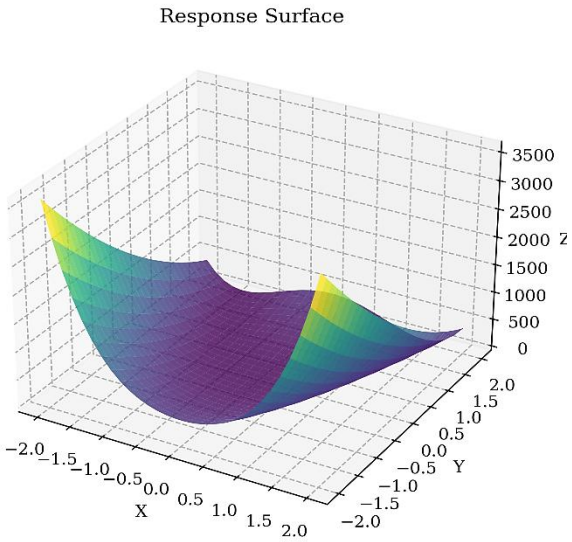


Fig. 2. Retained generic response-surface illustration.

The plotted surface is not accompanied by reactor equations, physical variables or units and must not be read as a chemical reaction model (*Fig. 2*).

4.1 | Evolutionary Algorithms

Genetic search can represent discrete choices using problem-specific variation [1]. DE operates naturally on continuous vectors [3], while CMA-ES adapts a continuous search distribution [8]. Their use in a reactor model requires operators and constraint treatment compatible with the engineering variables. Mixed variables or expensive model calls can change both feasibility and computational cost.

A local solver can be combined with a global search, or a surrogate can reduce expensive simulator calls. Such hybridization is a design option, not evidence of superiority. A credible comparison must count the local refinement, surrogate training and true model evaluations, and must confirm proposed solutions using the original physical model.

4.2 | Swarm Intelligence

PSO retains personal and shared best states [2], ABC allocates search around candidate food sources [4], and GWO, WOA and HHO use their respective candidate-update and selection mechanisms[5–7]. A metaphorical description is not a substitute for the implemented equations, parameter settings and constraint-handling code.

Continuous swarm positions must be mapped carefully when a reactor problem includes discrete equipment or integer decisions. Rounding can create repeated candidates, violate coupled constraints or change the effective search budget. A repair procedure should therefore be documented and its physical feasibility checked independently.

4.3 | Physics- and Bio-Inspired Methods

Other trajectory-based, physics-inspired and biological search frameworks may also be evaluated. Their labels do not determine suitability. For a reactor application, the relevant questions are which variables they manipulate, how they preserve feasibility and how many reliable simulator calls they require to produce a candidate.

Adaptive operators and surrogate-assisted evaluation are useful directions when objective calls are expensive. Adaptation itself introduces choices about rewards, training samples and stopping. Every auxiliary stage must be included in cost and validation accounting; otherwise a reported optimizer improvement may be caused by unequal information or compute.

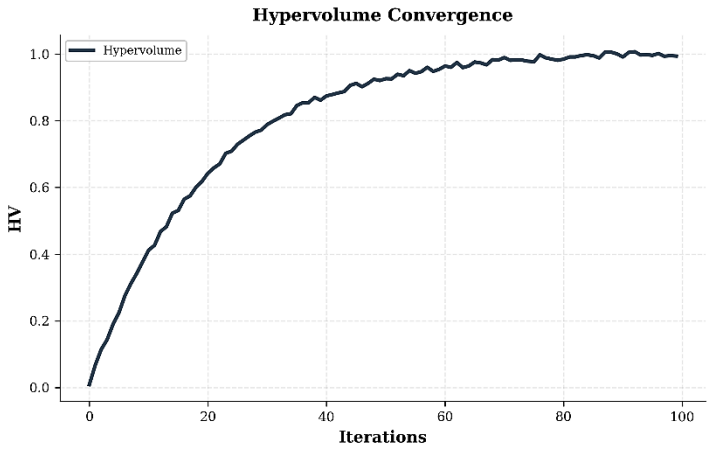


Fig. 3. Retained hypervolume convergence illustration.

Objective scaling, reference point, benchmark, budgets and run outputs are not specified; it does not establish a reactor pareto-front comparison (*Fig. 3*).

5 | Applications

Reactor design, process operation and control have different evidential requirements. Offline design can allow long simulations, while online control must return feasible actions within a deadline. Neither requirement can be inferred from a generic optimization benchmark.

5.1 | Primary Application Areas

The reactor literature includes competing production, economic, environmental, safety, energy and exergy objectives [9]. A multi-objective formulation must define the objective units and directions, the feasible region and the preferences used to select among candidates. Scalar weighted sums and Pareto approximation address different decisions and should not be described interchangeably.

Hybrid models can combine mechanistic balances with data-based components. A surrogate fitted on simulated samples is not independent physical validation, and extrapolation near unsafe operating regions requires particular care. An optimizer must not exploit numerical artifacts, unphysical model states or an inadequately trained surrogate to report a favorable objective.

Translating a selected point into operation requires checking it against the physical simulator, model-parameter uncertainty, actuator limits and relevant operating scenarios. Safety and real-time feasibility need explicit constraints and evidence. No particular algorithm family is certified for reactor deployment by this narrative.

Table 2. Retained qualitative algorithm descriptors.

Algorithm	Convergence	Robustness	Scalability	Ease of Use
PSO	Fast	Medium	Good	High
GA	Medium	Good	Good	High
DE	Fast	Good	Good	Medium
GWO	Fast	Good	Medium	High
WOA	Medium	Medium	Medium	High
ACO	Medium	Good	Medium	Medium
CMA-ES	Slow	Excellent	Poor	Low
SHADE	Fast	Excellent	Good	Medium

Note: Labels depend on the problem, implementation and budget; they are not measurements, universal rankings or aggregate findings from a verified reactor corpus.

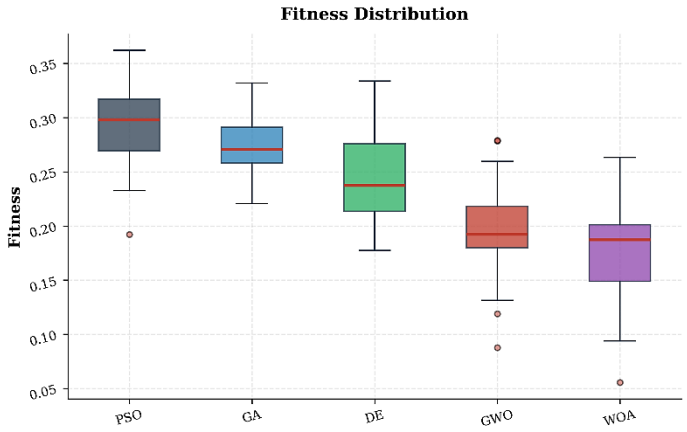


Fig. 4. Retained distributions of final fitness values across a reported 30 runs.

The objective, benchmark, constraints, paired seeds and execution logs are unspecified; the plot is not reactor-specific performance validation (*Fig. 4*).

6 | Challenges and Limitations

The central validity limits concern the physical model, algorithm budget and traceability of literature and experiments. These limits determine which engineering claims are warranted.

6.1 | Parameter Tuning

Tuning can materially affect a search method. An experimental protocol should state the ranges, trials, stopping rules and data or benchmark instances used to choose settings. Tuning budgets belong to the total cost, and configuration selection should remain separate from final evaluation. Covariance adaptation [8] does not make CMA-ES free of design choices.

6.2 | Benchmark Fairness and Reproducibility

Fair comparison requires identical problem instances, feasible domains and model tolerances, together with transparent objective-call and wall-clock budgets. Population size and generations are insufficient when methods use different numbers of trial evaluations. Raw per-run outputs, source code, simulator versions and seeds make both algorithm and physical-model errors inspectable.

6.3 | Theoretical Analysis and Scalability

Finite stochastic experiments do not prove global convergence. Theoretical claims need hypotheses about the feasible set, update process, evaluation error and acceptance law. Computational scalability must include simulator cost, constraint checks, sorting and surrogate fitting, rather than only vector updates.

Statistical tests must match their observational unit [10], [11]. The signed-rank test addresses paired differences; rank-sum tests concern independent samples. Friedman comparisons use multiple meaningful problem blocks, with post-hoc multiplicity control. Repeated runs of one reactor configuration quantify search randomness rather than the diversity of reactor problems. Effect sizes and confidence intervals should be reported with a justified dependence model.

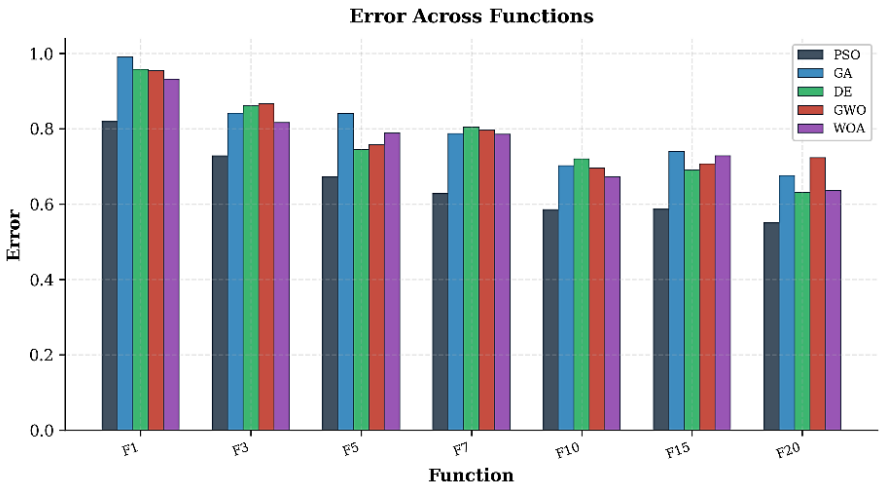


Fig. 5. Retained mean-error benchmark comparison.

Functions, error definition, aggregation and execution provenance are not supplied, so the figure cannot support a chemical reactor optimizer ranking (*Fig. 5*).

7 | Future Research Directions

Future studies should prioritize engineering evidence and reproducible computation before expanding the list of named algorithms.

Surrogate-assisted optimization is promising when reactor evaluation is costly. Its value must be assessed by true simulator calls and error near the selected operating point. Learning-based operator selection can also be studied, provided its training tasks are distinct from final test tasks and its overhead is counted.

Online applications need time-limited search, fallback actions and feasibility checks. Distributed computation may increase throughput but also changes communication cost and numerical consistency. Quantum-inspired representations remain classical computational designs unless a quantum resource is actually used; their names alone establish no engineering advantage.

A useful shared reactor benchmark would publish physical equations or a redistributable simulator, parameter domains and units, constraints, failure conventions, reference solutions and complete execution outputs. Multi-objective studies should also disclose reference points and objective normalization. These materials would make differences among optimizers interpretable.

Reproducibility extends to the review itself. Exact search logs, a deduplicated study register and study-by-study extraction are necessary before publication counts or historical trends can be reported. Energy use and execution cost can be evaluated when measurements exist, but no sustainability benefit should be inferred merely from fewer iterations.

8 | Conclusion

This perspective examined methodological requirements for metaheuristic reactor and process optimization. The central connection is between a physical formulation, a compatible search representation and an evaluation capable of checking feasibility, cost and performance. Its documentary record does not substantiate an exhaustive 179-paper review or the final-selection count 554, and its generic figures do not establish reactor-specific experiments.

Algorithm choice should follow problem structure, constraints and evaluation cost. Statistical conclusions require appropriate paired or independent units and control of multiplicity [10], [11]. Hybridization and newer update rules are options to test, rather than reasons to presume superiority. Physical validation and traceable simulation are necessary before selected configurations guide reactor operation.

The next evidential step is to reconcile the review register, replace unsupported trend claims with study-linked analysis and recover the provenance of the retained plots. A reactor-specific synthesis can then compare methods within compatible formulations and budgets. Until that evidence is available, the manuscript supports methodological discussion rather than a comprehensive empirical ranking.

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Data Availability

Sufficient data is available upon request.

Conflict of Interest

No potential conflict of interest was reported by the authors.

Consent for Publication

All authors have provided their consent for the publication of this manuscript.

Ethics Approval and Consent to Participate

This article does not involve studies with human participants or animals conducted by any authors.

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