

Data-Driven Optimization of Complex Engineering Operations

Dr. Emily Richardson

Assistant Professor, University of Waikato, New Zealand

Abstract

Complex engineering operations increasingly depend on interconnected processes, heterogeneous equipment, continuous data generation, and dynamic operational conditions. Conventional optimization approaches frequently rely on static assumptions, manually defined parameters, or simplified mathematical models that may not adequately represent the nonlinear relationships and uncertainty present in modern engineering environments. Data-driven optimization provides an alternative approach by combining operational data, statistical analysis, machine learning, predictive modeling, simulation, and optimization algorithms to improve engineering decision-making. This paper examines the role of data-driven methods in optimizing complex engineering operations, with particular attention to predictive analytics, intelligent resource allocation, process optimization, condition monitoring, scheduling, and adaptive decision-making. A conceptual analytical methodology is adopted to examine how data acquisition, preprocessing, analytical modeling, optimization, and feedback mechanisms contribute to operational improvement.

The analysis indicates that data-driven optimization can enhance resource utilization, process efficiency, equipment performance, operational reliability, and decision responsiveness by identifying patterns that may not be captured through conventional analytical methods. Machine learning can provide predictive insights, while optimization algorithms can use these insights to identify more efficient operational configurations. However, the effectiveness of data-driven optimization depends on data quality, model reliability, computational resources, system interoperability, and the representativeness of historical information. Important challenges include incomplete data, noisy measurements, model interpretability, changing operational conditions, cybersecurity, computational complexity, and integration with legacy engineering systems. Future research opportunities include digital twins, reinforcement learning, edge intelligence, explainable AI, federated optimization, autonomous engineering operations, and sustainability-aware decision models. The study concludes that data-driven optimization can provide a strong foundation for improving complex engineering operations when analytical intelligence is integrated with engineering knowledge, reliable data infrastructure, operational constraints, and continuous validation.

Keywords: Data-Driven Optimization; Engineering Operations; Machine Learning; Predictive Analytics; Operational Efficiency; Intelligent Decision-Making; Engineering Systems; Process Optimization; Digital Twins; Industrial Analytics

1. Introduction

Engineering operations have become increasingly complex as modern systems integrate advanced machinery, automated processes, interconnected sensors, digital platforms, and geographically

distributed resources. Manufacturing facilities, energy systems, transportation networks, infrastructure assets, and industrial processes generate large volumes of operational data that can provide valuable information about system behavior. However, the availability of data alone does not guarantee improved decision-making. Engineering organizations require analytical methods capable of converting heterogeneous operational information into actionable insights and optimized decisions.

Traditional engineering optimization frequently relies on mathematical models, predefined assumptions, expert knowledge, and historical operating parameters. These approaches remain important for many applications, particularly when physical relationships are well understood. Nevertheless, highly complex systems may contain nonlinear interactions, uncertain variables, changing environmental conditions, and large numbers of interdependent parameters. Data-driven approaches can complement traditional modeling by identifying patterns directly from observed system behavior and providing predictive information for operational decisions.

Machine learning and statistical analytics have expanded the capabilities of engineering optimization. Predictive models can estimate equipment conditions, production demand, energy consumption, system performance, or potential operational failures. Optimization algorithms can then use these predictions to determine resource allocations, production schedules, maintenance strategies, or operating parameters. This combination creates a feedback-oriented approach in which data continuously informs operational decisions.

The development of industrial Internet of Things technologies has further strengthened data-driven engineering. Sensors can collect real-time measurements from machines and processes, while communication networks transfer information to edge or cloud computing environments. Data-processing systems can transform these measurements into structured datasets, which can then be analyzed using machine learning and optimization techniques. This architecture enables engineering operations to become more responsive to current system conditions rather than relying exclusively on predetermined plans.

Despite its potential, data-driven optimization introduces several technical and organizational challenges. Historical datasets may contain missing observations, measurement errors, biased samples, or limited representations of abnormal conditions. Engineering systems can also change over time because of equipment aging, process modifications, environmental variation, and changing operating requirements. A model developed under one set of conditions may therefore become less reliable when applied to another. This paper examines the role of data-driven optimization in complex engineering operations, analyzes its major technological components, discusses implementation challenges, and identifies future directions for intelligent engineering decision-making.

2. Objectives

The primary objective of this study is to examine how data-driven methods can improve optimization and decision-making in complex engineering operations. The study focuses on the integration of operational data, machine learning, predictive analytics, optimization algorithms, and feedback mechanisms to improve efficiency, reliability, resource utilization, and operational responsiveness.

2.1 Evaluation of Data-Driven Optimization Approaches

The first objective is to evaluate analytical approaches used for data-driven engineering optimization. Machine learning, statistical modeling, predictive analytics, simulation, and mathematical optimization are examined according to their ability to support complex operational decisions.

The objective also considers the integration of historical and real-time data. Combining these sources can enable engineering systems to identify long-term operational patterns while responding to current conditions. Such integration is important for optimization problems involving changing workloads, equipment conditions, environmental factors, and resource constraints.

2.2 Assessment of Operational Efficiency

The second objective is to assess the contribution of data-driven optimization to major engineering performance indicators. Resource utilization, production efficiency, equipment reliability, energy consumption, process stability, and decision speed are considered important dimensions.

The study further examines factors that determine successful implementation. Data quality, model accuracy, computational efficiency, interoperability, cybersecurity, and engineering expertise are treated as important conditions for achieving reliable optimization outcomes.

3. Literature Review

3.1 Data-Driven Engineering and Smart Manufacturing

Data-driven engineering has become increasingly important with the growth of digital sensing, industrial connectivity, and computational analytics. Kusiak emphasized the role of data and intelligent technologies in smart manufacturing, while Tao et al. highlighted the increasing importance of data-driven approaches for production systems. These studies demonstrate that manufacturing and engineering decisions can increasingly be supported by continuously generated operational information.

Data-driven methods are particularly useful when complex physical relationships are difficult to model explicitly. Rather than depending exclusively on predefined equations, machine learning methods can identify statistical relationships between process variables and operational outcomes. However, such approaches should complement rather than completely replace physical engineering knowledge, particularly when safety, reliability, and regulatory constraints are important.

3.2 Machine Learning for Engineering Optimization

Machine learning provides predictive capabilities that can support engineering optimization. Supervised learning models can estimate performance outcomes from historical data, while unsupervised methods can identify hidden patterns and operational states. Deep learning can process high-dimensional data, including images, sensor signals, and sequential measurements.

Optimization can then be performed using predictions generated by analytical models. For example, a predictive model can estimate equipment degradation while an optimization algorithm determines maintenance timing. Similarly, demand prediction can support production scheduling and resource allocation. This interaction between prediction and optimization is a central feature of data-driven engineering operations.

3.3 Digital Twins and Simulation-Based Optimization

Digital twins provide another important foundation for data-driven engineering optimization. Tao et al. described digital twins as virtual representations of physical systems that can integrate data, models, and simulation capabilities. Such environments allow engineers to evaluate operational changes before applying them to physical systems.

Simulation can also provide additional information when historical data are insufficient. By combining physical models with observed operational data, engineering organizations can evaluate

alternative scenarios and identify potentially improved operating conditions. This can reduce the risks associated with direct experimentation on complex physical systems.

4. Methodology

4.1 Research Design

This study adopts a conceptual analytical research design to examine data-driven optimization of complex engineering operations. The methodology synthesizes research related to machine learning, industrial analytics, optimization, cyber-physical systems, digital twins, predictive maintenance, and smart engineering.

The research treats data-driven optimization as an iterative process involving data acquisition, preprocessing, prediction, optimization, implementation, monitoring, and feedback. This structure recognizes that optimization is not a one-time computational activity but an ongoing process in which operational information continuously influences engineering decisions.

4.2 Data Acquisition and Preparation

Engineering data can originate from sensors, machines, enterprise systems, maintenance records, production databases, environmental monitoring systems, and operational logs. These data may differ in format, frequency, accuracy, and scale. Effective optimization therefore requires data integration and appropriate preprocessing before analytical models are developed.

Data preparation may include noise reduction, missing-value treatment, normalization, synchronization, feature engineering, and anomaly identification. The methodology also considers the importance of maintaining temporal relationships within engineering datasets. Data leakage and inappropriate sampling can lead to unrealistic model performance and should therefore be carefully controlled.

4.3 Predictive and Optimization Analysis

The study examines the integration of predictive models with optimization methods.

Key analytical dimensions include:

- Predictive performance
- Resource allocation
- Process optimization
- Production scheduling
- Equipment condition estimation
- Energy optimization
- Operational risk assessment
- Real-time decision support
- Model adaptability

Predictive models provide estimates of future or unobserved conditions, while optimization methods identify operational decisions that maximize desired objectives subject to engineering constraints.

4.4 Performance and Validation

Data-driven optimization systems should be evaluated using both predictive and operational indicators. Model-level measures may include prediction error, precision, recall, and robustness, while operational measures may include productivity, resource utilization, downtime, energy consumption, and cost.

Validation should also consider changing operational conditions. A model that performs well on historical data may not provide equivalent results under new conditions. Cross-validation, temporal testing, scenario analysis, simulation, and real-world pilot studies can provide stronger evidence of model reliability.

5. Analysis

5.1 Data-Driven Optimization Architecture

A data-driven engineering optimization system typically consists of multiple interconnected layers. The sensing layer collects operational information, the data layer stores and preprocesses measurements, and the analytical layer generates predictions and identifies patterns. An optimization layer then determines appropriate operational decisions, which are implemented through engineering control or management systems.

This architecture creates a feedback loop between physical operations and analytical models. New operational data can be used to evaluate previous decisions and update predictive models. Such continuous feedback can make optimization more adaptive than static planning approaches.

Table 1: Components of Data-Driven Engineering Optimization

Component	Primary Function	Optimization Contribution
Sensors	Capture operational conditions	Provides real-time information
Data Infrastructure	Stores and manages data	Enables analytical accessibility
Data Preprocessing	Improves data quality	Reduces analytical errors
Machine Learning	Identifies patterns and predicts outcomes	Supports informed decisions
Optimization Algorithms	Selects suitable operating decisions	Improves resource allocation
Simulation	Evaluates alternative scenarios	Reduces implementation risk
Digital Twins	Represents physical systems digitally	Enables predictive optimization
Control Systems	Executes operational decisions	Converts optimization into action
Monitoring	Tracks outcomes	Supports continuous improvement

Interpretation: Table 1 shows that data-driven optimization requires an integrated architecture rather than a standalone machine learning model. Sensors and data infrastructure provide the information foundation, while analytical models generate predictions. Optimization algorithms translate those predictions into decisions, and control systems implement them.

Monitoring completes the feedback loop by evaluating outcomes. The integration of these components enables engineering operations to move toward continuous, evidence-based optimization.

5.2 Operational Performance Optimization

Data-driven optimization can improve engineering performance by identifying relationships between operational parameters and desired outcomes. For example, production systems can optimize machine settings according to quality and throughput requirements, while energy systems can adjust resource usage according to demand patterns. Equipment management can similarly use predictive information to optimize maintenance timing.

The effectiveness of optimization depends on the quality of both predictions and decision models. An inaccurate prediction can lead to an inappropriate optimization decision, while an optimization algorithm that ignores engineering constraints may produce impractical solutions. Therefore, data-driven optimization must incorporate technical, operational, and safety constraints.

Table 2: Engineering Performance Areas Supported by Data-Driven Optimization

Performance Area	Data-Driven Mechanism	Potential Outcome
Production Efficiency	Predictive process optimization	Improved throughput
Resource Utilization	Intelligent allocation	Reduced resource waste
Equipment Reliability	Condition prediction	Reduced unexpected downtime
Energy Management	Demand and consumption analysis	Improved energy efficiency
Scheduling	Predictive demand analysis	Better production coordination
Quality Control	Pattern detection	Improved quality consistency
Maintenance	Failure-risk prediction	More effective maintenance timing
Process Stability	Continuous monitoring	Faster deviation response
Decision Speed	Automated analytics	Faster operational decisions

Interpretation: Table 2 demonstrates that data-driven optimization can influence multiple dimensions of engineering performance. Predictive analytics can improve production planning and maintenance decisions, while resource and energy optimization can reduce unnecessary consumption.

Automated quality analysis can improve consistency, and continuous monitoring can support faster responses to deviations. However, these outcomes depend on reliable data and well-designed optimization objectives. The most effective systems therefore combine predictive intelligence with explicit operational constraints and engineering expertise.

5.3 Real-Time Engineering Decision-Making

Real-time data-driven optimization can enable engineering organizations to respond more rapidly to changing operational conditions. Instead of waiting for periodic reports, automated systems can continuously evaluate process data and identify deviations or emerging opportunities for optimization.

Edge computing can support time-sensitive decisions by processing information near the source. Cloud platforms can provide broader computational resources for historical analysis, model training, and large-scale optimization. Hybrid architectures can therefore combine rapid local decision-making with centralized analytical capabilities.

6. Discussion

6.1 Integration of Prediction and Optimization

The integration of predictive analytics with optimization provides a major advantage for complex engineering operations. Prediction identifies what may happen under current or future conditions, while optimization determines what action should be taken. Together, these capabilities can support more proactive decisions than conventional reactive approaches. However, prediction uncertainty must be considered during optimization. A decision based on a highly uncertain forecast may create operational risk. Robust and uncertainty-aware optimization methods can therefore improve the reliability of data-driven engineering decisions.

6.2 Adaptability to Changing Conditions

Engineering operations rarely remain completely static. Equipment aging, changing production schedules, environmental variation, material differences, and evolving operational objectives can alter relationships between inputs and outcomes. Data-driven models must therefore remain adaptable. Continuous monitoring can identify changes in model behavior, while retraining and online learning can update predictive capabilities. However, uncontrolled model adaptation can also introduce unexpected behavior. Model updates should therefore be validated and governed carefully, particularly in safety-sensitive engineering environments.

6.3 Engineering Knowledge and Data Intelligence

Although data-driven methods can identify patterns that are difficult to model manually, engineering knowledge remains essential. Physical constraints, safety requirements, process relationships, and domain-specific operating limits cannot always be inferred reliably from historical data. The most effective optimization frameworks are therefore likely to combine data-driven models with physics-based knowledge and expert constraints. This hybrid approach can improve interpretability, reduce unrealistic decisions, and provide stronger generalization when historical data are incomplete or changing.

7. Challenges

7.1 Data Quality and Availability

Engineering datasets frequently contain missing values, sensor errors, inconsistent sampling, and incomplete records. Fault events may also be underrepresented because reliable engineering systems are designed to avoid failures. These characteristics can limit the ability of machine learning models to learn rare or important operational conditions.

Data-quality management, sensor validation, data augmentation, simulation, and appropriate sampling strategies are therefore important. Organizations must also establish consistent data-management practices to maintain analytical reliability over time.

7.2 Model Generalization and Interpretability

A model trained on historical engineering data may perform poorly when operating conditions change. This is particularly challenging when equipment is modified, environmental conditions shift, or new products are introduced. Model interpretability is another concern because engineering teams may require explanations before accepting automated optimization recommendations.

Explainable AI, uncertainty estimation, transfer learning, and domain adaptation can improve trust and generalization. Nevertheless, these methods must be validated using realistic engineering scenarios rather than relying only on theoretical evaluations.

7.3 Computational and Integration Complexity

Complex optimization problems may require significant computational resources, particularly when they involve large datasets, many variables, or real-time constraints. Integrating analytical systems with legacy engineering infrastructure can further increase implementation complexity. Communication delays can also reduce the effectiveness of real-time optimization.

Edge computing, cloud infrastructure, modular software architectures, and efficient algorithms can help address these challenges. However, organizations must balance computational sophistication with reliability, maintainability, and operational requirements.

8. Future Research

8.1 Reinforcement Learning for Engineering Optimization

Future research can investigate reinforcement learning for adaptive engineering optimization. Reinforcement learning systems can learn operational policies through repeated interactions with simulated or controlled environments. This capability may allow systems to optimize complex processes where conventional mathematical models are difficult to construct.

However, safe exploration remains essential because inappropriate actions can damage equipment or affect production. Research should therefore emphasize constrained reinforcement learning, simulation-based training, uncertainty management, and safe transfer from digital environments to physical engineering systems.

8.2 Digital Twins and Autonomous Optimization

Digital twins can provide a valuable environment for testing data-driven optimization strategies before physical implementation. Future systems could continuously synchronize digital representations with physical assets and use them to evaluate alternative operating decisions.

This could support autonomous optimization of production, maintenance, energy consumption, and resource allocation. Research should investigate efficient synchronization, real-time model updating, uncertainty representation, and scalable digital-twin architectures. Integration with AI could enable increasingly autonomous engineering operations while maintaining controlled physical constraints.

8.3 Edge Intelligence and Federated Optimization

Future engineering systems may distribute optimization capabilities across edge devices, local industrial systems, and centralized platforms. Edge intelligence can reduce latency and support rapid operational responses, while federated approaches can enable multiple engineering sites to learn from distributed information without necessarily centralizing sensitive operational datasets.

Research should examine communication efficiency, privacy, model consistency, and distributed optimization strategies. Such architectures could support large-scale engineering networks while improving responsiveness and data governance.

9. Limitations

This study adopts a conceptual analytical approach and does not introduce a newly collected engineering dataset or conduct experimental optimization within a specific industrial facility. Consequently, the identified benefits represent generalized relationships supported by existing research rather than direct measurements from a controlled operational environment.

The study also does not compare specific machine learning algorithms, optimization solvers, or commercial engineering platforms through standardized benchmarking. Performance may vary considerably according to application characteristics, data availability, computational infrastructure, and operational constraints. Future research should therefore conduct empirical evaluations across multiple engineering domains and compare data-driven approaches under realistic operating conditions.

10. Conclusion

Data-driven optimization provides an important approach for improving complex engineering operations by connecting operational data with predictive analytics, optimization algorithms, simulation, and intelligent decision-making. Continuous sensor information can reveal patterns in equipment behavior, production performance, energy consumption, and resource utilization that may be difficult to identify through conventional approaches. When predictive models are combined with optimization mechanisms, engineering organizations can move from reactive decision-making toward more proactive and adaptive operational management.

The analysis demonstrates that successful data-driven optimization depends on an integrated architecture. Sensors, data infrastructure, preprocessing systems, machine learning models, optimization algorithms, control systems, and monitoring mechanisms must operate together. Improvements in production efficiency, equipment reliability, quality, energy management, and resource utilization require reliable data and carefully defined optimization objectives. Engineering expertise remains essential for establishing physical constraints, validating predictions, and ensuring that automated decisions remain safe and operationally feasible.

Future engineering operations are likely to become increasingly autonomous, connected, and adaptive. Reinforcement learning, digital twins, edge intelligence, federated optimization, explainable AI, and hybrid physics-data models can provide new capabilities for intelligent optimization. These technologies can enable engineering systems to continuously learn from operational information while adapting to changing conditions. When implemented with strong validation, cybersecurity, governance, and engineering oversight, data-driven optimization can contribute substantially to more efficient, reliable, flexible, and sustainable engineering operations.

References

1. Du, S., Huang, Z., Jin, L., & Wan, X. (2024). Recent progress in data-driven intelligent modeling and optimization algorithms for industrial processes. *Algorithms*, 17(12), 569. <https://doi.org/10.3390/a17120569>
2. Lawrence, N. P., Damarla, S. K., Kim, J. W., Tulsyan, A., Amjad, F., Wang, K., Chachuat, B., Lee, J. M., Huang, B., & Gopaluni, R. B. (2024). Machine learning for industrial sensing and control: A

- survey and practical perspective. *Control Engineering Practice*, 145, 105841. <https://doi.org/10.1016/j.conengprac.2024.105841>
3. Paraschos, P. D., & Koulouriotis, D. E. (2024). Learning-based production, maintenance, and quality optimization in smart manufacturing systems: A literature review and trends. *Computers & Industrial Engineering*, 198, 110656. <https://doi.org/10.1016/j.cie.2024.110656>
 4. Chen, H., Zhang, Z., Li, W., Liu, Q., Sun, K., Fan, D., & Cui, W. (2024). Ensemble of surrogates in black-box-type engineering optimization: Recent advances and applications. *Expert Systems with Applications*, 248, 123427. <https://doi.org/10.1016/j.eswa.2024.123427>
 5. Houssein, E. H., Saeed, M. K., Hu, G., & Al-Sayed, M. M. (2024). Metaheuristics for solving global and engineering optimization problems: Review, applications, open issues and challenges. *Archives of Computational Methods in Engineering*, 31, 4485–4519. <https://doi.org/10.1007/s11831-024-10168-6>
 6. Di Fiore, F., Nardelli, M., & Mainini, L. (2024). Active learning and Bayesian optimization: A unified perspective to learn with a goal. *Archives of Computational Methods in Engineering*, 31, 2985–3013. <https://doi.org/10.1007/s11831-024-10064-z>
 7. Azevedo, B. F., Rocha, A. M. A. C., & Pereira, A. I. (2024). Hybrid approaches to optimization and machine learning methods: A systematic literature review. *Machine Learning*, 113, 4055–4097. <https://doi.org/10.1007/s10994-023-06467-x>
 8. Liu, S., Wang, H., Peng, W., & Yao, W. (2024). Surrogate-assisted evolutionary algorithms for expensive combinatorial optimization: A survey. *Complex & Intelligent Systems*, 10, 5933–5949. <https://doi.org/10.1007/s40747-024-01465-5>
 9. Ouahabi, N., Chebak, A., Kamach, O., Laayati, O., & Zegrari, M. (2024). Leveraging digital twin into dynamic production scheduling: A review. *Robotics and Computer-Integrated Manufacturing*, 89, 102778. <https://doi.org/10.1016/j.rcim.2024.102778>
 10. Eichenseer, P., & Winkler, H. (2024). A data-oriented shopfloor management in the production context: A systematic literature review. *The International Journal of Advanced Manufacturing Technology*, 134, 4071–4097. <https://doi.org/10.1007/s00170-024-14238-8>
 11. Abdel-Aty, T. A., & Negri, E. (2024). Conceptualizing the digital thread for smart manufacturing: A systematic literature review. *Journal of Intelligent Manufacturing*, 35, 3629–3653. <https://doi.org/10.1007/s10845-024-02407-1>
 12. Song, J., Cui, Y., Wei, P., Valdebenito, M. A., & Zhang, W. (2024). Constrained Bayesian optimization algorithms for estimating design points in structural reliability analysis. *Reliability Engineering & System Safety*, 241, 109613. <https://doi.org/10.1016/j.ress.2023.109613>
 13. Pelamatti, J., Le Riche, R., Helbert, C., & Blanchet-Scalliet, C. (2024). Coupling and selecting constraints in Bayesian optimization under uncertainties. *Optimization and Engineering*, 25, 373–412. <https://doi.org/10.1007/s11081-023-09807-x>
 14. van de Berg, D., Savage, T., Petsagkourakis, P., Zhang, D., Shah, N., & del Rio-Chanona, E. A. (2022). Data-driven optimization for process systems engineering applications. *Chemical Engineering Science*, 248, 117135. <https://doi.org/10.1016/j.ces.2021.117135>
 15. Daoutidis, P., Lee, J. H., Rangarajan, S., Chiang, L., Gopaluni, B., Schweidtmann, A. M., Harjunkoski, I., Mercangöz, M., Mesbah, A., Boukouvala, F., Lima, F. V., del Rio Chanona, A., & Georgakis, C. (2024). Machine learning in process systems engineering: Challenges and opportunities. *Computers & Chemical Engineering*, 181, 108523. <https://doi.org/10.1016/j.compchemeng.2023.108523>

16. Bishnu, S. K., Alnouri, S. Y., & Al-Mohannadi, D. M. (2023). Computational applications using data driven modeling in process systems: A review. *Digital Chemical Engineering*, 8, 100111. <https://doi.org/10.1016/j.dche.2023.100111>
17. Yang, M., Jiang, P., Zang, T., & Liu, Y. (2023). Data-driven intelligent computational design for products: Method, techniques, and applications. *Journal of Computational Design and Engineering*, 10(4), 1561–1578. <https://doi.org/10.1093/jcde/qwad070>
18. He, C., Zhang, Y., Gong, D., & Ji, X. (2023). A review of surrogate-assisted evolutionary algorithms for expensive optimization problems. *Expert Systems with Applications*, 217, 119495. <https://doi.org/10.1016/j.eswa.2022.119495>
19. Wang, X., Jin, Y., Schmitt, S., & Olhofer, M. (2023). Recent advances in Bayesian optimization. *ACM Computing Surveys*, 55(13s), Article 287, 1–36. <https://doi.org/10.1145/3582078>
20. Fisher, O. J., Watson, N. J., Escrig, J. E., Witt, R., Porcu, L., Bacon, D., Rigley, M., & Gomes, R. L. (2020). Considerations, challenges and opportunities when developing data-driven models for process manufacturing systems. *Computers & Chemical Engineering*, 140, 106881. <https://doi.org/10.1016/j.compchemeng.2020.106881>