Machine Learning for Efficient CFD-based Quantitative Risk Analysis: Progress and Practical Insights

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1. Introduction

In chemical process industry, the presence of large quantities of hazardous materials necessitates quantitative risk assessment (QRA) as a powerful tool for reducing risks. QRA is a systematic approach to evaluate risk levels, probabilities, and consequences of hazardous events in complex technological systems (Arora et al., 2021). Over the decades, regulatory bodies worldwide have established many QRA standards and guidelines (American Institute of Chemical Engineers, 2007; Health and Safety Executive (HSE), 2001; European Union Directive, 2012; API, 2016), providing frameworks to systematically evaluate and mitigate risks from hazardous processes. As pointed out by Apostolakis (2004), QRA is not simply about “getting the number right”, it is the impact on decision-making that matters. In order to understand how the system can fail and to prevent such events, both academia and industry are actively developing new methodologies and tools to enhance the robustness of QRA.

A key component of QRA is analysing the consequences of accidents such as fires, explosions, and hazardous substances releases, which can provide high level of confidence in results and robust justification for risk-based decision making, if done adequately (UNECE, 2023). Traditionally, consequence analysis methods often rely on integral models, which are usually fast and easy-to-implement, but may often oversimplify the physics of complex scenarios (Mannan, 2012; Pappalardo et al., 2021). This limitation has driven the increasing use of computational fluid dynamics (CFD) in modelling accident effects in these cases.

In recent years, advancements in high-performance computing have significantly enhanced the feasibility of deploying CFD for consequence analysis in geometrically complex industrial environments (Runchal and Rao, 2020). Shen et al. (2020) systematically reviewed the application of CFD in consequence analysis for the process industries, demonstrating its implementation in fire, explosion, and hazardous material dispersion modelling with improved predictive capabilities compared to traditional methods. However, the time-consuming nature of CFD persists as a critical barrier to its widespread adoption in QRAs.

Recent advances in machine learning (ML) offer strategies to mitigate the computational burden of CFD, this integration can enhance CFD through accelerating direct numerical simulations (DNS), improving turbulence models, and developing reduced-order models (ROM) (Vinuesa and Brunton, 2022). Existing reviews have explored ML’s role in enhancing CFD (Caron et al., 2025; Panchigar et al., 2022; Rahman et al., 2024) and its adaptability across various domains of safety and reliability (Tamascelli et al., 2024). Nonetheless, the specific use of ML-accelerated CFD in the context of QRA –especially in complex industrial settings– has not been thoroughly examined.

This extended abstract reviews diverse strategies for integrating ML with CFD to enhance QRA in process industry, with a focus on recent progress in balancing the efficiency and accuracy regarding the consequence modelling in complex environments. To address the importance of introducing ML into this framework, challenges and current practices regarding the use of CFD in QRA are discussed based on results from an online survey presented in Section 2. ML’s ability to streamline CFD processes for QRA is analysed and compared in detail through a literature review in Section 3. Finally, conclusions and future research trends are given in Section 4.

2. Challenges in CFD-based QRA

While the role of CFD tools in consequence analysis is very clear, their contribution in the entire QRA framework is less addressed in the literature. In fact, CFD tools are much more computationally expensive than those simplified integral models, thus limiting the practical application in QRAs (Patel et al., 2024). To better understand the practical application of CFD in QRA, the authors conducted an anonymous survey examining the stages, scenarios, and conditions under which CFD is utilized, as well as the challenges faced in its application.

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| (a) Work fields of the participants. | (b) Frequency of using CFD compared to other models during QRAs. |
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| (c) Key challenges in using CFD for QRA. | |
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| (d) Conditions for choosing CFD over simpler models. | |

Figure 1: Survey results.

The survey was publicized through two main channels: direct emails were sent to domain experts and colleagues with relevant experience in risk assessment and CFD, and the survey was also shared publicly via LinkedIn posts to engage a broader professional audience involved in safety engineering, process design, and regulatory bodies. A total of 24 responses were collected, of which 20 participants had either directly used CFD or observed its use in QRA projects. As shown in Figure 1 (a), the majority of respondents (42%) identified as working in academia, while the rest were from industry or regulatory bodies, reflecting a diverse perspective on CFD practices across sectors. The survey revealed that most participants (75%) believe CFD is used less frequently than simpler models in QRA workflows, as illustrated in Figure 1 (b). This was attributed primarily to high computational cost, technical complexity, tight project timelines, and the difficulty of model validation (Figure 1 (c)). The reason for respondents to choose CFD over simpler models, as shown in Figure 1 (d), is primarily due to the presence of complex geometries, high-consequence scenarios, or regulatory requirements. These findings are consistent with observations in the literature, where the benefits of CFD in terms of accuracy and detail are often constrained by practical usability and resource limitations, thus hindering its broader adoption. Other insights from the survey include preferred CFD software tools, such as ANSYS Fluent, FLACS, and FDS, and the typical project phases where CFD is applied –most commonly during detailed design or post–incident analysis. Respondents also shared the specific types of risk scenarios modelled using CFD through a multiple-choice question, with fire (70%), explosion (65%), and gas dispersion (55%) being the most frequent applications.

The survey results, aligned with existing literature (Patel et al., 2024; Shen et al., 2020), highlight key barriers of using CFD in QRA. Most notably the high computational cost, the ease of use and validation challenges significantly restrict the routine application of CFD in the QRA. In order to adress these issues, the next section reviews how ML techniques are being integrated with CFD to overcome these specific barriers.

3. ML-CFD integration strategies for efficient QRA

This section presents a purpose-driven overview of how ML has been integrated with CFD to improve its applicability in QRA. Recent research efforts are grouped into three main purposes that reflect the needs of QRA practice: 1) surrogate modelling and acceleration, 2) parameter and model calibration, and 3) real-time prediction. Some relevant areas of each category are listed in Table 1. Despite some overlaps, note that the technical implementation of ML algorithms is beyond the scope of this work, as the structure aims to reflect practical utility in risk assessment.

Table 1: Relevant areas of ML-CFD integration strategies for QRA.

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| Surrogate modelling and acceleration | Parameter and model calibration | Real-time prediction |
| Reduced-order models | ML-enhanced turbulence closures | Digital twins |
| Regression-based surrogates | Uncertainty quantification | Sensor-data integration |
| Dimensionality reduction | Bayesian parameter optimization | Physics-informed neural networks (PINNs) |
| Physics-informed surrogate models | Data assimilation for model refinement |

3.1 Surrogate modelling and acceleration

To make CFD more feasible within risk-based frameworks, many recent studies have focused on constructing surrogate models that approximate high-fidelity simulations at a fraction of the cost. Early works (Loy et al., 2017, 2018) demonstrated the potential of support vector machines and interpolation-based models to estimate net radiation flux from LNG pool fires, enabling faster consequence assessments in facility design and siting. Similar surrogate strategies have been adopted in explosion modelling. For example, Jung and Shin (2024) trained an XGBoost model on FLACS simulation data to predict overpressures from hydrogen leaks, showing excellent accuracy and speed suitable for scenario screening in QRA.

More advanced approaches integrate dimensionality reduction and deep learning. Burela et al. (2025) combined POD-based (Proper Orthogonal Decomposition) reduction with neural networks to simulate wildfire spread, achieving near-instant front prediction, offering promising solutions for the consequence analysis of Natech (Natural Hazard Triggering Technological Accidents) scenarios. Kashefi et al. (2021) developed a novel point-cloud deep learning approach that directly predicts flow fields around complex geometries by processing unstructured mesh vertices, enabling accurate predictions for unseen shapes while maintaining physical conservation laws. Abrate et al. (2023) proposed a bootstrapped POD-RBF (Radial Basis Function) model for offshore gas releases, cutting simulation time by orders of magnitude with minimal error. Meanwhile, Usman et al. (2021) applied deep learning to accelerate large-eddy simulations of atmospheric dispersion, achieving fast and generalizable plume predictions across different source terms and conditions.

In parallel, physics-informed neural networks (PINNs) have emerged as an alternative way to build surrogates that embed governing equations directly into the training process. Comparing to conventional data-driven approaches, PINNs are especially effective for inverse problems and data-scarce scenarios where traditional supervised learning struggles (Wong et al., 2021). Several studies highlight their potential: PINNs have shown up to 25% improvement in accuracy over data-driven approaches (Donnelly et al., 2024), achieved speedups of up to fivefold compared to conventional CFD solvers (Ang and Ng, 2022), and even reduced computational effort by a factor of eight (Sousa et al., 2024). Studies by Wang et al. (2021) and Fernández et al. (2023) further illustrate their potential as lightweight, generalizable CFD surrogates, while limitations such as training instability and accuracy degradation still exist. As surrogate modelling techniques continue to evolve, combining data-driven learning with physical constraints and uncertainty estimation will be key in fluid dynamics simulations and risk analysis.

3.2 Parameter and model calibration

Turbulence modelling remains one of the most challenging aspects of CFD, particularly in the context of Reynolds-Averaged Navier–Stokes (RANS) and Large Eddy Simulation (LES) approaches (Vinuesa and Brunton, 2022). The integration of ML and turbulence modelling has shown the potential in overcoming the limitations of conventional closure models. Instead of relying solely on empirical coefficients or fixed eddy-viscosity formulations, recent studies have explored learning turbulence behavior directly from high-fidelity data. For instance, Maulik et al. (2021) developed surrogate models for turbulent eddy viscosity in RANS, enabling steady-state solutions by accelerating convergence by a factor of 5. While Ling et al. (2016) introduced a tensor-basis neural network (TBNN) to model Reynolds stress in a way that respects physical invariances. These approaches enhance the expressiveness of RANS models, especially in flow regions where traditional closures fail. The PINN-based frameworks proposed by Zhou et al. (2024) and Jang et al. (2024) further offer flexible alternatives by embedding the governing equations directly into the training process, bypassing the need for explicit turbulence models in certain scenarios.

Uncertainty quantification and model calibration are also gaining attention, particularly through Bayesian methods. Maruyama et al. (2021) used Bayesian inference to infer turbulence model coefficients and quantify uncertainty using limited experimental data, demonstrating improved prediction and reliability for CFD applications. Similarly, Both et al. (2019) proposed a surrogate-assisted Bayesian optimization approach to calibrate model parameters using explosion test data. For system-level modeling, Berghe et al. (2023) proposed a machine learning framework to calibrate parameters in reduced-order ejector models by combining data-driven and physics-integrated approaches These techniques not only improve model fidelity but also help quantify the confidence bounds of predictions, providing valuable inputs for risk assessment frameworks.

These above-mentioned studies show that ML-enhanced parameter and model calibration have potential to make CFD more accurate, adaptive, and uncertainty-aware —three qualities that are essential for advancing consequence modeling and scenario analysis in QRA. Future work will need to further explore model transferability, hybrid learning strategies, and the integration of real-time data for continuous model refinement.

3.3 Real-time prediction

The demand for real-time consequence assessment in dynamic risk scenarios has driven increasing interest in integrating machine learning with CFD for fast and adaptive predictions. Digital Twins represent a new paradigm in computational modelling, where ML is used to expand CFD simulation databases for rapid response across a wide range of operational conditions. This hybrid physics-informed and data-driven approach, termed simulation digital twin (SDT), enables real-time prediction and decision support (Molinaro et al., 2021). Thomas et al. (2021) developed accelerated digital twins using lattice Boltzmann algorithms and graphics card-based computing to predict real-time fluid mechanics in mixing tanks, providing insights into stratified two-fluid mixing processes.

Another emerging research focus is sensor-driven integration, which connects physical systems with computational models to enhance real-time monitoring and predictive capabilities. Kim et al. (2019) combined long short-term memory recurrent neural network (LSTM-RNN) with CFD simulations to accurately localize hazardous material leaks in chemical plants using sparse sensor inputs, by training on CFD-generated datasets. Similarly, Li et al. (2024) developed a deep probabilistic learning model for real-time hydrogen dispersion prediction, emphasizing uncertainty estimation and boundary accuracy, which could support future digital twin implementations for emergency management. Also focused on real-time hydrogen leak monitoring at hydrogen refueling stations (HRS), Wang et al. (2024) proposed another regression model based on temporal convolutional networks (TCN) and multimodal sensor fusion, by integrating wind and concentration data, it outperforms conventional models like LSTM, offering guidance for sensor layout and provide a reliable real-time solution for large-scale HRS safety monitoring.

Besides the widely adoption of PINNs in surrogate modelling and parameter calibration, in the comprehensive survey on ML for CFD (H. Wang et al., 2024), PINNs are also highlighted as a key methodology for solving inverse problems while maintaining physical consistency. For example, Shi et al. (2023) integrated variational Bayesian inference with deep learning to predict spatial explosion overpressures in offshore platforms, achieving real-time accuracy (R² = 0.955) by combining sparse sensor data with physics-based constraints. These integrations enable rapid and reliable risk assessment such as flammable gas leaks and explosions, thus allowing real-time decision-making with improved efficiency.

4. Conclusions

This review summarized the current state of integrating ML techniques with CFD for enhancing QRA in process industry. Focusing on three application-driven categories: surrogate modelling and acceleration, parameter and model calibration, and real-time prediction, we identified representative studies, categorized typical ML approaches, and discussed their relevance to key QRA challenges such as simulation cost, model uncertainty, and decision-making speed.

It is found that methods such as surrogate modelling and parameter optimization show promise in balancing computational efficiency and predictive rigor, meanwhile ML-facilitated real-time prediction can provide valuable insights for dynamic risk assessment. Despite its potential, the integration of ML and CFD in QRA still faces challenges such as insufficient high-quality training data, compatibility issues across software tools, and the case-specific nature in terms of complex environments. Future research trends include establishing shared CFD databases, exploring real-time risk assessment frameworks and promoting industry standards to ensure the reliability of ML-CFD in QRA.

Acknowledgments

The authors thank the survey respondents for their insights on CFD applications in QRA. This work was done in the framework of Project 101119358, ‘PROSAFE’, funded by the Marie Skłodowska-Curie Actions programme, HORIZON-MSCA-2022-DN-01. A. This work was also partly funded by Grant PID2023-150607OB-I00 funded by MICIU/AEI/ 10.13039/501100011033 and by ERDF/EU.

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