ProSafe: Smart Integration of Process Systems Engineering & Machine Learning for Improved Process Safety

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1. Introduction

ProSafe is a novel interdisciplinary initiative (Figure 1) aiming to make a step change and reinforce the process safety effectiveness with new methods and skills exploiting emerging digital transformation opportunities (Big Data, ML, AI) in alignment with the EU digitalization roadmap of the European manufacturing industry initiative.

A diagram of a company's process

AI-generated content may be incorrect.

Figure 1. Integration of the doctoral candidates (DCs) into the research program.

Successful process safety enhancement in high-hazard industries calls for the development of new high-level process safety research. In this regard, the synergy between process safety, process systems engineering, machine learning, and artificial intelligence, which is usurping the new era of industry, has not yet been exploited. The underlying reasons are, among others, segregated research, and development efforts at different academic and non-academic centers in EU combined with the complexity of the problem, which makes it too big to tackle alone with a single discipline/research center. Thus, there is a strong need for a European doctoral training program bringing together complementary disciplines in research and training, which sets the motivation for ProSafe.

* + 1. Project objectives

ProSafe aims to bring together a critical mass of partners with interdisciplinary expertise and competencies to undertake original research and train next-generation engineers able to combine machine learning, artificial intelligence, and process systems engineering with domain knowledge of process industry and process safety, to significantly improve safety and productivity in high hazard industries. ProSafe will pioneer new foundations by integrating Quantitative Risk Assessment (QRA), Process Systems Engineering (PSE) (model-based approach) with interpretable machine learning (ML) and artificial intelligence (AI) disciplines (data- and knowledge-based approaches) as targeted breakthroughs to achieve the objectives. Through this research and training program, ProSafe will contribute to realizing the promising potential of the new artificial intelligence paradigm with a particular focus on process safety. To this end, ProSafe will develop new synergistic tools and train skilled professionals to address this very important societal, economic, and environmental challenge of safe and sustainable process industries. In the next section the ***research objectives (RO), training objectives (TO),*** and their associated WPs (Table 3.1a) are described.

* + 1. Research Objectives (RO)
* **RO1:** Harmonize robust QRA methods and implementation strategies for effective and improved risk assessment and process safety (from model to improved process risk assessment and safety; top-down approach) (WP2).
* **RO2:** Develop AI and ML (especially interpretable ML) models using domain knowledge for efficient, safe, and reliable process operations (from data to improved process, operation, and safety; bottom-up approach) (WP3)
* **RO3:** Develop synergistic integration of model-based with data-based methods for improved process safety operation and monitoring (from model & data to improved process safety; a hybrid approach) (WP4).
* **RO4:** Identify roadmap and efficient implementation strategies for AI and ML for improved process operation and safety: demonstration and validation of ProSafe novel concepts and methods (RO1, RO2, RO3) on industrial relevant case studies for safer operation (WP5).
  + 1. Training Objectives (TO)
* **TO1:** Training of DCs through individual projects combining multidisciplinary competencies in AI, ML, and PSE within the domain of process safety (WP2-5).
* **TO2:** Create a new generation of multidisciplinary professionals to pioneer new process safety for the future digital industry: Recruit top candidates with a strategic blend of scientific backgrounds from engineering to AI/ML disciplines (WP1).
* **TO3:** Establish and pilot the concept of a truly interdisciplinary European multicenter training program in AI/ML, QRA, and PSE areas within the domain of safety in process industries through relevant network-wide events, courses, workshops, and on-site industry training that complement training in soft skills for effective communication and entrepreneurship (WP6).

By realizing the ambitious training and research objectives, ProSafe is expected to have a transformative impact on the larger sector of European process industries and reinforce their competitiveness thanks to timely alignment with the broader transformation of European process industries under the Industry 4.0 trend.

* + 1. ProSafe Consortium

This multidisciplinary consortium comprises a complementary set of 1) university departments very active in research on Hazard identification and quantitative risk analysis (UPC), process systems engineering (DTU, NTNU, KU, COL), process control and automation (DTU, NTNU, KU, COL), Computer Science and model-based AI (IMPERIAL, COL), Machine learning/Big Data analytics (IMPERIAL, DTU, NTNU, KU, COL), Open science practices (IMPERIAL) and 2) non-academic partners within process and plant operation from high hazard process industries (PdB), industrial QRA engineering providers (NOVOTEC, RISKTEC), software providers for process safety (KAIROS), process risk management and safety training (RISKTEC). Thus, we cover the full range of academic skills needed to advance the tools, training, and implementation required to upgrade the performance of risk analysis and monitoring, operation and maintenance planning in an integrated way, and the range of developers, service users, and clients to define, validate and exploit the research questions and outputs.

Table 1: ProSafe Consortium composition

|  |  |  |
| --- | --- | --- |
| Partner | Name | Country |
| 1 (Coordinator) | Technical University of Denmark (DTU) | Denmark |
| 2 | Universitat Politecnica De Catalunya (UPC) | Spain |
| 3 | Norwegian University of Science and Technology (NTNU) | Norway |
| 4 | Novotec Consultores SA (NOVOTEC) | Spain |
| 5 | Koç University (KU) | Turkey |
| 6 | Kairos Technology (KAIROS) | Denmark |
| 7 | Risktec Solutions (RISKTEC) | UK |
| 8 | Port de Barcelona (PdB) | Spain |
| 9 | Columbia University | USA |
| 10 | Imperial College London (IMPERIAL) | UK |

* 1. Methods
     1. Overall methodology

PROSAFE´s research program divides the 12 doctoral student projects into 4 technical WPs. The interrelation between the WPs (see Figure 1) is as follows: in WP2, the doctoral candidate (DC) projects (1, 5, 8, 9) contribute to the advancement of the model-based methods by leveraging QRA with PSE methods for harmonized and robust quantitative risk assessment for improving safety; inWP3, the DC projects (4, 6, 7, 11, 12), focus primarily on the systematic study of the data for safety approach by developing neuro-symbolic learning methods that exploit domain knowledge and AI/ML algorithms for online risk monitoring and safe process operation; in WP4, the DC projects (2, 3, 10) undertake research for synergistic integration of model-based with data-based methods (WP3) for improved process safety; in WP5, the research of DC projects converges in three themes to demonstrate and test improved process safety on selected cases from multi-sectorial industries (e.g., urea, LNG, renewable hydrogen). WP5 will provide the platform for the cross-fertilization of different ideas and concepts for interactive and synergistic improvement and validation of new methods and skills from model-based, data-driven, and hybrid approaches. In this way, PROSAFE overcomes the disadvantages associated with each separate approach. Indeed, the model-based approach relies on first principles and mechanistic modeling of systems dynamics, which makes them often overly reductive given the complexity of the problem. On the other hand, data-based approaches (such as AI and ML) very much depend on the quantity and quality of the data (as in garbage in =garbage out), which may not necessarily be available in sufficient context to enable complete system description and knowledge. Therefore, through smart hybrid integration and recent advancements in data and knowledge-driven ML technologies, ProSafe presents a powerful and complementary research program for DC students to undertake cutting-edge research. The research has also a promising potential and relevance to reinforce safer process operations in alignment with the needs of future digital process industries.

* + 1. Integration of methods and disciplines

The research methodology is based on combining top-down and bottom-up approaches to comprehensively address complex aspects of process safety challenges.

* ***In our top-down approach***, we go from model to improved process safety, in which we employ model-based methods that are used in QRA and PSE domains to identify and evaluate risk, make better decisions, and develop methods for improved risk assessment and process safety (WP2).
* ***In our bottom-up approach***, we go from data to improved process safety (WP3). We build upon and expand the knowledge and understanding of risk achieved in top-down methods (WP2) with data-driven methods, employing both numeric AI and knowledge-driven symbolic ML (WP3).
* ***In the hybrid approach***, we combine a model-based approach (WP2) with a data-based approach (WP3) to study the synergistic integration of these approaches for improved understanding and mitigation of process safety risks in high-hazard process industries (WP4).

The integration of these approaches and disciplines will be demonstrated with three high-hazard industry sectors (WP5). These case studies will be crosslinked with interdisciplinary work on model-based (WP2), data-based (WP3), and the synergistic integration of these into hybrid approaches (WP4). DCs working on the same case study but cutting across multiple WPs (e.g., DC-1, -7, -2) will benefit from exchange with the other DCs working on that system, as they use each other’s experience along with industrial partner’s expertise for optimal interaction within the given case study. DCs working on the same approach but on different case studies (e.g., DC-7, -4, -6) will develop joint solutions to cross-cutting challenges and learn to exploit various elements and systems for developing new methods and tools tailored to the scope and the needs of that specific process safety domain. Various process safety insights generated by each DC project from a multi-disciplinary approach will be discussed and exchanged between DC students during workshops (see training by research) regularly to ensure cross-fertilization and synergy among different projects.

3. DCs contributions to the ProSafe research program

DCs projects are expected to contribute to the research program per WPs as follows:

**WP2 Model-based foundation for improved risk assessment & process safety (model to improved safety):** WP2 aims to significantly advance the tools and methods for effective and improved risk assessment and process safety using model-based methods. DC-1 will develop an efficient methodology to predict and propagate the model output uncertainty in risk criteria estimation in QRA. By performing a comprehensive uncertainty and sensitivity analysis and including the sources of uncertainties, DC-1 will evaluate their impact on QRA results and propose measures for robustifying the methodology. DC-5 will develop a framework for benchmark analysis and selection of QRA models to ensure consistency in their application to assess major accident effects. DC-8 will use CFD tools together with new accident mathematical models to improve consequence analysis in QRA studies and DC-9 will develop a methodology to perform QRA, which will make use of improved mathematical models to quantify the effects of major accidents on hydrogen facilities. DC-1 and -5 will work in close collaboration to improve the QRA methodologies, as well as DC-5 and -8 to improve consequences assessment. DC-9 will in part make use of the results from the previous DCs to apply them to hydrogen facilities specifically. Results from DC-5 and -8 will also be used by DC-6 to fill the cause and consequences database.

**WP3 Artificial intelligence/machine learning for risk monitoring and safe process operation (data to improved safety):** WP3 aims to develop neuro-symbolic solutions that integrate data-driven concepts, frameworks, and technologies based on deep learning and symbolic ML, to provide big data science for risk monitoring and safe process operation underpinned by established domain knowledge. For this DC-4 will design numeric AI (deep learning algorithms) to develop novel predictive analytics for online risk monitoring and fault diagnosis. DC-6 will develop a hybrid, regressible, and robust ML methodology that identifies abnormal events, and integrates process phenomenological knowledge and historical data. DC-7 will complement DC-6 with physics-informed machine learning algorithms tailored to control chemical processes. DC-11 will apply advanced symbolic ML methods to learn interpretable models of cause and effects of faults and abnormal behaviors that can be used to predict deviations from normal operation and establish a platform for early detection of abnormal events during plant operation. DC-12 will use inputs from DC-4 (online risk monitoring) and DC-11 (online detection of abnormal events) to develop an efficient online neuro-symbolic ML for predicting the consequences of abnormal events and diagnostics in terms of likely causes and related mitigation. Output from DC-4, -11, and -12 will be used for the definition of major hazard scenarios among others as part of the development of the harmonized QRA methods in WP2.

**WP4 Hybrid approaches and tools integration (model & data to improved safety):** WP4 focuses on the synergistic and smart integration of model-based and data-driven methods for improved process safety (RO3). For that, DC-2 will develop a novel hybrid modeling framework for risk monitoring that combines model-based algorithms with ML algorithms. DC-2 works in close collaboration with DC-4 to bridge the gap between model-based and data-based approaches for safety. DC-3 contributes through the design of novel algorithms for short-term optimal operation by using robust model predictive control, state estimation, and risk monitoring methods. DC-10 contributes through the integration of knowledge-based models with data-driven online learning to build a long-term prognostic model framework for planned maintenance in plants. DC-10 works in close collaboration with DC-3 to build prognostic degradation models.

**WP5 Domain applications to selected high hazards multisector process industries:** This WP focuses on comprehensive testing, validation, and evaluation of the ambitious and new process safety concepts and methods developed by the doctoral students on selected case studies from high-risk industries as defined in RO4. Thus, all DC projects contribute to this WP. More specifically, DC-1, -7, and -2 will test and validate the urea case studies together with RISKTEC as the relevant industry partner. DC-4, -5, -9, and -10 will work on the regasification plant and other energy vectors distribution (such as ammonia and methanol) in collaboration with Port de Barcelona as the industry partner. Finally, we will use hydrogen production as a case study to test and validate methods and tools developed by DC-3, -6, and - 8 in collaboration with Kairos as the relevant industry partner. Overall, this ensures that the methods and tools from WP2, 3, and 4 are tested iteratively and validated across three sectors comprehensively.

4. Conclusions

ProSafe network undertakes innovative and original research and offers unique multi-sectorial and multi-disciplinary research and training opportunities for a total of 12 doctoral candidates (DCs) in the disciplines of machine learning (ML), artificial intelligence (AI), and process systems engineering (PSE) with domain knowledge of process industry and process safety.

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References

<https://prosafe.dtu.dk/>

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