SSM
Scuola Superiore Meridionale

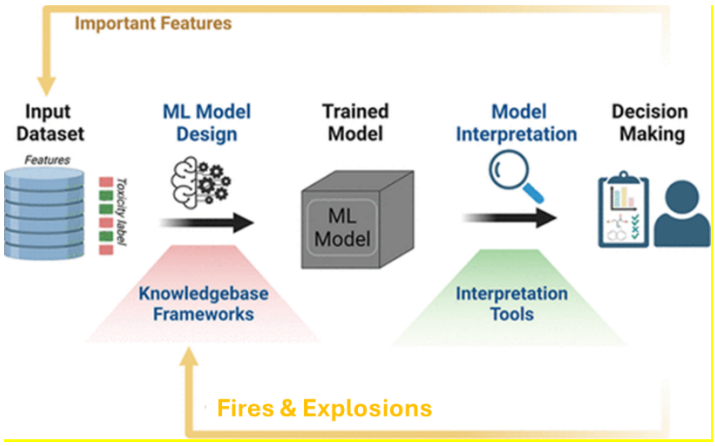
MERC PhD Project Proposal 2024/2025

AI-aided Risk Analysis in Chemical Industry

Project description

Risk analysis and quantitative risk assessment is crucial in the chemical industry in order to design units and processes which are safe and sustainable by design.
They are crucial steps in any chemical process and operation development and they often represent a legal requirement.
However, up to date risk analysis is still based on a combination of historical data analysis, semi-empirical models, and tacit and heuristic knowledge by human experts. Most of these are based on traditional chemical industry development and often inadequate to describe the new challenges and transformations of the chemical industry for a sustainable future.
For instance, the shift from a carbon-based energetic/chemical industry to a sustainable hydrogen economy poses serious safety issues, not entirely addressed by the available risk analysis tools. Hydrogen has unique properties compared to traditional fossils, making available semi-empirical models inadequate for hydrogen dispersion and incidental scenarios consequences.
Many other analogous examples can be found in most renewable processes, from electrocatalytic fuel synthesis and utilization, to biomass exploitation.
Contemporary scientific literature is attempting to address the challenges by using artificial intelligence techniques, machine learning and surrogate modelling to gain the unavailable knowledge and parameters.
The attempts are promising but the peculiarities of the application field pose many challenges and require many research efforts in adapting traditional machine-learning algorithms and methodologies.
Experimental data in industrial safety can be scarce and sparse, so less employed surrogate models such as gaussian processes can be adopted to deal with the specifics of the available data. Moreover, a combination of high-computational-cost simulations, such as CFD simulations and ab-initio properties predictions, is necessary to integrate the available knowledge and allow surrogates to efficiently navigate the variable space to give significant results.
Data scarcity can be also addressed by combining these approaches with the most promising hybrid modelling techniques, taking into account both incomplete available physical models and surrogate-based statistical techniques.

The key question of this project is: **can we use a combination of statistical machine-learning techniques, hybrid semi-empirical models, and physical computational models to make risk analysis more accurate, fast, and flexible to address the safety issues of an ever-changing chemical industry?**



OBJECTIVES

The main aim of the project proposal is the development a general methodology to apply machine learning techniques in combination with traditional risk analysis tools in order to address specific challenges of renewable and green processes.

The specific objectives are described in the following.

Objective 1 – Identification of significant case studies in the field of renewable chemical processes to address with hybrid machine learning techniques.

Objective 2 – Integration of machine learning algorithms with available inadequate semi-empirical models and scarce experimental data, to bridge the gap between the peculiarities of the field of chemical safety and the traditional ML surrogates.

Objective 3 – Advancement in consequence modelling and risk analysis performed on selected case studies based on the development methodology and model validation through available experimental data and result of high-computational-cost simulations.

METHODOLOGIES

To achieve the above objectives, the research project is organized in Tasks.

Task1 – Case studies definition and literature systematization

Open challenges in the field of renewable chemical industry will be identified based on the available data-set for property predictions, historical safety data, and consequence analysis tools. Data will be collected and rationalized to identify the specifics machine learning approaches to address the specifics of the field.

Task2 – Hybrid-machine-learning modelling for risk identification

Based on the results of the previous task, available semi-empirical models will be merged with machine learning methods in order to predict the unknown parameters based on the available data-sets and the results of physical models, such as CFD and ab-initio property predictions. Less

explored machine learning tools will be adopted, such as Gaussian-Processes-based surrogates. These are proven to be more interpretable, flexible with scarce data-sets, can give a clear estimation of uncertainties. The underpinning idea use a hybrid combination of interpretable ML techniques with available physical and semi-empirical models in order to overcome one of the main limitations of traditional ML approaches, such as the black-box problem solving approach making it extremely challenging to interpret the results and transfer them through different scales and applications.

Task3 – Model validation

The objective will be to adopt high-fidelity CFD simulations and available experimental data not used for the training to validate the predictions of the developed models also transferring the developed methodology to analogous yet different case studies.
This will be achieved by data-driven construction of reduced order models of ODEs and PDEs from CDF simulations and data and the construction of the appropriate closures for the detailed physical models for comparison and validation.

Relevance to the MERC PhD Program

The proposed project deals with Risk in Industrial Processes and also to Complexity, as it will be performed by the development of advanced models (CFD and Machine Learning).

The disciplines relevant to this project are the following:

1) *Risk analysis – engineering, analysis and management of risks*

Procedure and tools for performing risk analysis is multidisciplinary as it deals with consequence analysis ad frequency analysis.

2) *Machine learning - mathematical modelling and simulation of complex systems*

To perform consequence analysis the development of advanced models to simulate complex phenomena resulting from the interaction between turbulence and combustion is required.
The numerical and modelling complexity related to the development of models for unsteady turbulent combustion is a key factor in this project. Commitment on mathematical modelling and chemical/physical models of turbulent combustion flows and numerical issues will be demanding.

Key references

[1] Sansana J. et al., 2021. Computers and Chemical Engineering 151, 107365.
[2] Jiao Z. et al., 2020. ACS Chemical Health and Safety, 27, 6, 316 – 334.
[3] Hedge J and Rokseth B, 2020. Safety Science 122, 104492.

Joint supervision arrangements

Supervisors are:
Prof. Almerinda Di Benedetto – University of Naples Federico II will support the whole PhD activity.
Prof. Danilo Russo - University of Naples Federico II will support the activity based on the development of the Machine Learning based model.
Every 4 weeks the PhD student will meet with both supervisors.

Location and length of the study period abroad (min 12 months)

Agreement is in preparation.

Any other useful information

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