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Understanding industrial process dynamics through AI: the case of a recycle reactor process

Project n°4

01

Towards Trustworthy ML for Industrial Process Modelling

Context

1. Industrial Challenge

Complex, nonlinear and interconnected systems often controlled with PID loops

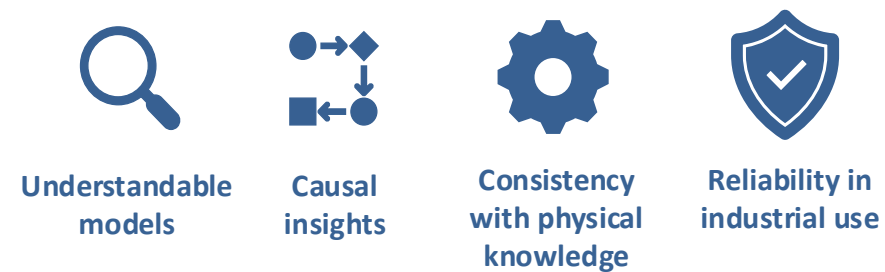


- Nonlinear dynamics
- Strong variable couplings
- Uncertainty, disturbances & faults
- Sub-optimal operation & economic losses

2. The Trust Gap

More and more ML methods are developed for industrial processes ...

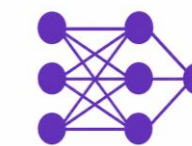
But their adoption critically depends on trust and interpretability



Industrial AI needs to be accurate, interpretable and trustworthy

3. Our Research Approach

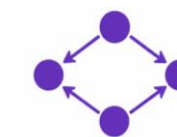
Compare four complementary modelling directions to build trustworthy models



Black-box ML with post-hoc Explainability
DNN, RNN, Transformers



Intrinsicly Interpretable Models
SINDy, KANs, TFT



Causal Modelling
Structural dynamical causal models

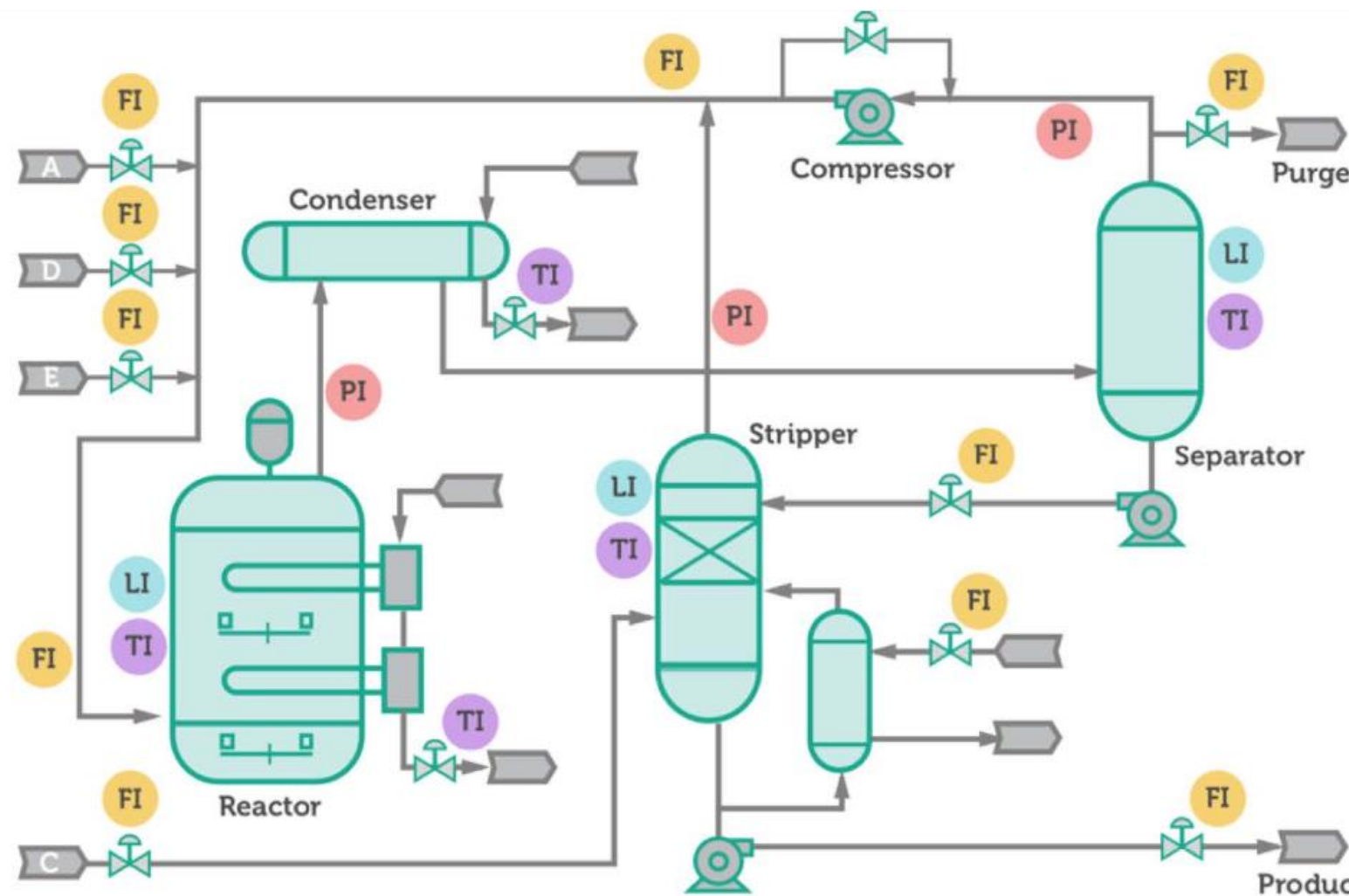
$$\frac{dx}{dt} = f(x, u)$$

Physics-informed Models
PINNs, state-space models

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Case study: Tennessee Eastman Process (TEP)

Context



41 measured process variables (XMEAS)



12 control variables (XMV)



Sample every 3 min – up to 25-48h



Includes normal & faulty operations



Widely used benchmark for control, monitoring & fault detection

Product 1 $A(g) + C(g) + D(g) \rightarrow G(liq)$ Product 2 $A(g) + C(g) + E(g) \rightarrow H(liq)$



GOAL: Develop and compare interpretable, causally meaningful and physics-consistent ML models for better monitoring, control and digital twin development in industrial environments.



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Founding Team

- **Noémie Vlaminc**
 - *Institution:* Cenaero
 - *Expertise:* Time series forecasting, manufacturing data analysis, computer vision, speech
- **Cyriac Delie**
 - *Institution:* ULiège
 - *Expertise:* Dynamical systems reconstruction, physics-based ML
- **Aysu Ozden**
 - *Institution:* Cenaero
 - *Expertise:* Multi-fidelity reduced-order modelling, digital twin
- **Zahra Zamanian**
 - *Institution:* UMONS
 - *Expertise:* Battery Management Systems, dynamical system control

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Work Plan

- **Dataset preparation**
 - Explore TEP dataset
 - Agree on preprocessing procedure
- **Predictive modelling baseline**
 - Train black-box models to get a baseline for comparison
- **First insight into model interpretability**
 - Apply post-hoc explainability techniques on baseline models: feature importance, sensitivity analysis, SHAP
- **Intrinsically interpretable models**
 - Exploration of methods like symbolic regression, KANs and Temporal Fusion Transformer
- **Causal Modelling**
 - Analysis of dependencies and potential causal graphs
 - Identification of key drivers in system dynamics
- **Hybrid physics-informed models**
 - Implementation of simplified physics-informed ML approaches: energy conservation constraints, PINN-inspired methods if feasible

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Expertise Sought

We are looking for people interested in going beyond black-box models by incorporating explainability, interpretability, causality, or physics-based knowledge into their AI methods.

- **Explainable & Interpretable AI**
 - Post-hoc interpretability techniques: SHAP, LIME, attention analysis, feature importance
 - Designing inherently interpretable models: symbolic regression, KANs
- **Causal Machine Learning**
 - Causal discovery & inference methods
- **Physics-informed AI**
 - PINNs and constraint-based learning
 - Integrating domain knowledge into ML pipelines: differential equations, conservation laws

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THANK YOU FOR YOUR ATTENTION !

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