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# CMLM: A Cascade of Machine Learning Models to detect and diagnose the performance of model predictive controllers

**Elizabeth V. Melo[a]*, Argimiro R. Secchi[ab], and Maurício B. de Souza Jr.[ab]**

[a] Chemical Engineering Program, PEQ/COPPE, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil
[b] EPQB, School of Chemistry, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil
* Corresponding Author: evmelo@peq.coppe.ufrj.br.

## ABSTRACT

In this work, we propose a methodology for monitoring the performance of model predictive controllers (MPCs). A sequence of binary classification machine learning models, organized in cascade, called Cascade Machine Learning Models (CMLM), is evaluated to give a diagnosis of the control conditions. The proposed methodology was assessed using two case studies: a benchmark problem (the van de Vusse reactor under nonlinear MPC, NMPC) and a simulated industrial debutanizer column under commercial MPC. The ML models evaluated were the Random Forest and the Multilayer Perceptron. The results show that the proposed approach outperforms both a single multiclass model and traditional MPC performance monitoring methodologies, while remaining adaptable and scalable to larger applications.

**Keywords**: Machine Learning, Artificial Intelligence, Nonlinear Model Predictive Control, Process Monitoring, Fault Detection

## INTRODUCTION

Model predictive controllers (MPCs) have become popular in industrial applications. However, just like other control strategies, this kind of controller depends on a healthy closed-loop configuration to perform properly. The satisfactory implementation of an MPC depends on its tuning parameters and mainly on the model representation, and a plant-model mismatch is still a challenge to be identified [1, 2].

Many metrics have been developed to detect and diagnose performance issues in controllers [3, 4]. Indeed, commercial software already has some tools to help monitor the closed-loop operation. However, obtaining a quick and accurate diagnosis remains challenging in industrial processes [5]. Improving data visualization is one of the approaches that has been explored for easing control loop diagnosis [6]. Machine learning (ML) is one of the classes of techniques employed to detect and diagnose control performance issues.

Control degradation is considered part of the fault detection and diagnosis (FDD) field [4], which is already widely exploring ML applications in abnormalities classification [6-8]. Some studies have been conducted to evaluate the applicability of ML tools in monitoring control loops, most of them focusing on SISO loops [10-13], and some on MPC [14-17]. However, there is still a lack of studies that evaluate the use of ML tools applied to nonlinear MPCs (NMPCs) and commercial MPCs.

In this study, we explore the use of ML algorithms applied to detect and diagnose the performance of MPCs. We propose a sequential procedure to evaluate the usage of independent ML models, named Cascade Machine Learning Models (CMLM), to detect and diagnose the performance of model predictive controllers using a data-based approach. To evaluate this approach, a comparison between Random Forest (RF) and Multilayer Perceptron (MLP) Neural Network as candidate ML models is carried out. As case studies, the van de Vusse reactor controlled by an NMPC, a nonlinear benchmark, and a simulated industrial debutanizer column controlled by a commercial MPC, with more variables involved, were used to generate data to train, validate, and test the learning capability of the ML models.

## METHODOLOGY

### System Architecture

Figure 1 shows a schematic representation of the process controlled by an (N)MPC and integrated with the AI-based monitoring system. This proposal aims to evaluate the capability of an IA agency to apply online to an industrial process, giving alerts and suggesting corrective actions to improve control performance.

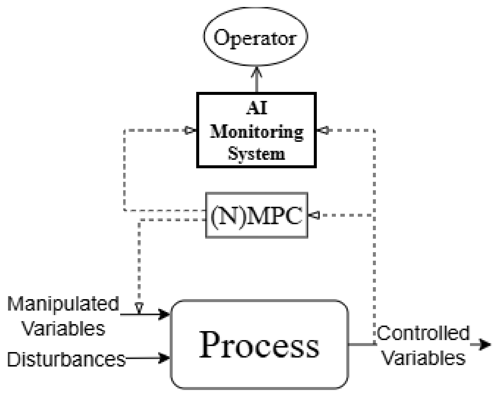



**Figure 1.** Controlled process integrated with the AI-based monitoring system.

### Models in Cascade

Models in cascade have already been used for monitoring MPC performance [15]. However, this methodology has not been widely explored, especially for NMPC's performance monitoring. Figure 2 illustrates how these ML models are organized for the van de Vusse reactor system, while Figure 3 shows how it was designed for the debutanizer column, the case studies of this work. The specific adaptation of the CMLM is based on the physical knowledge of the process and on the main typical source of degradation. Process particularities must be taken into consideration to design the cascade arrangement.

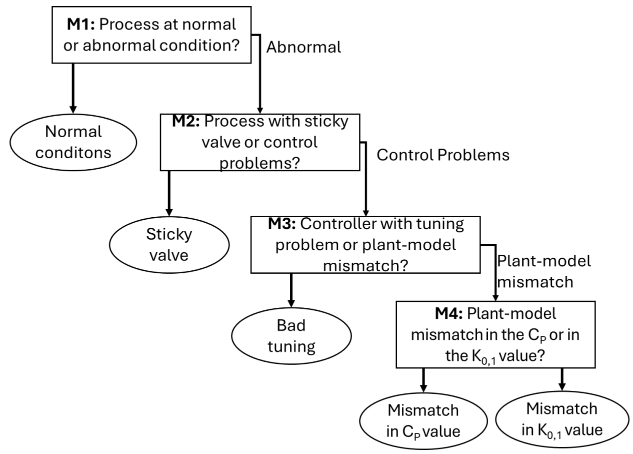



**Figure 2.** Models (M) in cascade for the classification problem for the van de Vusse reactor.

In Figure 2, the CMLM was designed to discriminate between the instrumentation and process problems and the control configuration problem. The first ML model is responsible for detecting whether the closed-loop performance is abnormal. Once abnormalities are detected, the process data goes to the second ML model, which is responsible for diagnosing whether the issue is due to the process actuator, such as valve stiction, or internal control configuration. Once an internal control

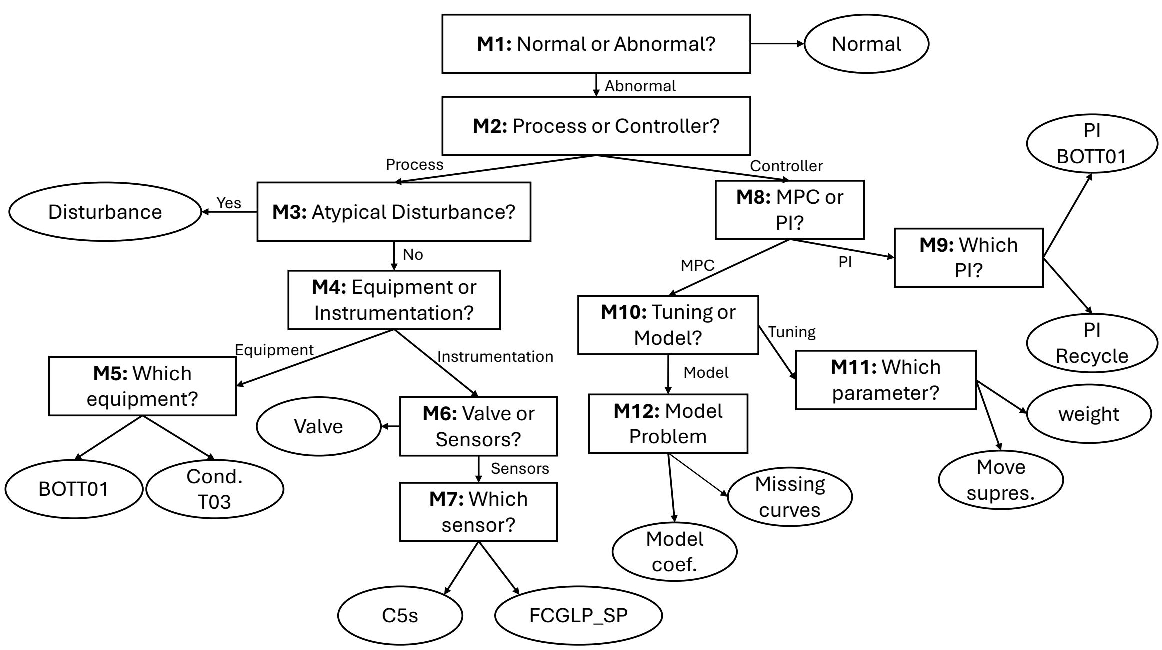
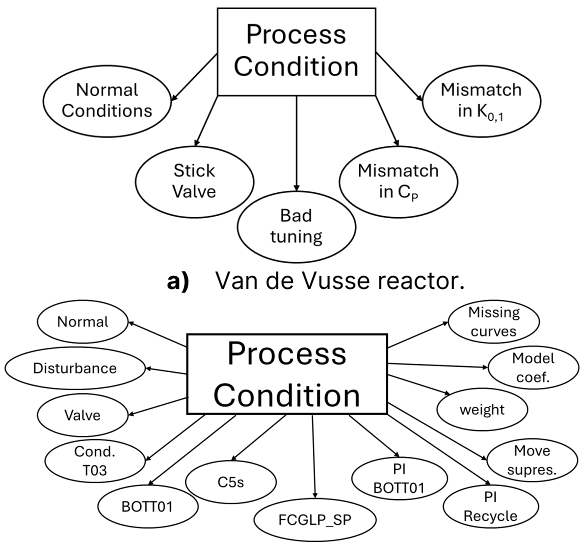



**Figure 3.** Models (M) in cascade for the classification problem for the debutanizer column.

configuration issue is detected, the third ML model is used for diagnosing poor control tuning or plant-model mismatch. Finally, if a plant-model mismatch is identified, the final model is responsible for diagnosing which of the two process model parameters should be evaluated.

The CMLM for the distillation column presented in Figure 3 follows, in general terms, its counterpart developed for the benchmark reactor. However, as the model is now more complex, additional models were included, such as M8 and M9, which deal with PI regulatory control. Additionally, to make the FDD problem more complete, models designed to detect atypical disturbances (M3) and sensor problems (M7) were also included.

This methodology is compared with a single machine learning model (SMLM) for a multiclass classification, in which detection and diagnosis occur at the same model, according to Figure 4. The multiclass approach is used in other studies for MPC status classification.




**a)** Van de Vusse reactor.

**b)** Debutanizer column.

**Figure 4.** ML representation for multiclass classification (diagnosis and detection) problem for each case study.

The main advantage of using CMLM is its facility for maintenance and adaptations. Chemical processes with many variables and controllers in cascade may suffer from a huge number of possible issues in the closed loop. In this case, there is a necessity to update the SMLM structure, and the whole model should be retrained, while the CMLM allows the possibility to update just one of the structures used or include a new model for a new diagnosis.

Besides, CMLM allows the use of different ML algorithms combined, as one technique can be better for one specific diagnosis than others. Furthermore, the technical team can also contribute to the precise diagnosis, removing models from the cascade. For example, if it is certain that the process is not under normal conditions, the operators and engineers can use only the models regarding the diagnosis, skipping the detection model.

Moreover, for each diagnosis, different features are expected to affect each abnormally. For the SMLM, all features that might contribute must be used, resulting in a complex ML model. For the CMLM, in case there is a necessity of reducing model complexity, different features could be used for each model in the cascade, allowing the construction of simpler models.

## Case Study 1: van de Vusse Reactor

To evaluate the CMLM methodology, the van de Vusse reactor was used as a case study. The reaction system produces a substance B from a reagent A, having C and D as byproducts, according to Equation (1).

$$A \xrightarrow{1} B \xrightarrow{2} C \quad 2A \xrightarrow{3} D \tag{1}$$

The inlet flow enters a CSTR reactor with a temperature $T_{in}$, a concentration $C_{A,in}$ of reagent A, and a flowrate $F$, according to Figure 5. The outlet B concentration ($C_B$) and the reactor temperature ($T$) are the controlled variables (CVs). The heat exchange rate $\dot{Q}$ and the flowrate and reactor volume ratio $F/V$ are used as manipulated variables (MVs). All system parameters were described by Engell and Klatt (1993) [18].

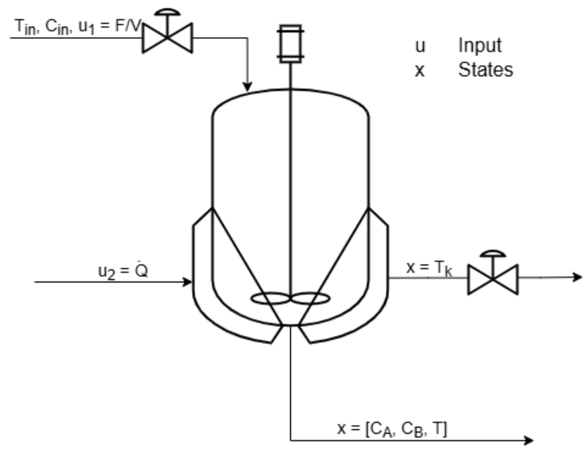



**Figure 5.** van de Vusse reactor.

The reactor is controlled by an NMPC. All simulations were run considering the same steady state as the initial process condition. The simulations were carried out using the same structure used by Lima *et al.* [19]. The concentration $C_{A,in}$ is considered an unmeasured disturbance. A sampling time of $2.5 \times 10^{-3}$ h was adopted.

### Data Generation

The simulation for generating the data was carried out considering four different cases:

1. **Normal conditions:** absence of faults.
2. **Valve stiction:** a dead band was considered.

3. **Poor tuning:** intentional poor tuning was made at the controller.

4. **Plant-model mismatch in $C_P$ or $K_{0,1}$:** difference between the NMPC internal model and the simulated plant for the specific heat of the mixture $C_P$ or for the pre-exponential constant of the B formation reaction rate ($K_{0,1}$) were considered.

Simulations were performed to produce 10, 000 samples for each class. The presence of Gaussian noise in the measurement of the control variables was also applied.

## Case Study 2: Debutanizer Column

The system is based on a Natural Gas Processing Unit (NGPU) that produces Liquefied Petroleum Gas (LPG) from Natural Gas. The system is composed of three distillation columns: a demethanizer, a deethanizer, and a debutanizer column. The main column is the debutanizer column, which processes the liquid from the bottom of the deethanizer to produce LPG and light naphtha.

Figure 6 shows the simplified scheme of the process. The simulation was carried out using Aspen Dynamics, controlled by DMC3, the AspenTech's controller.

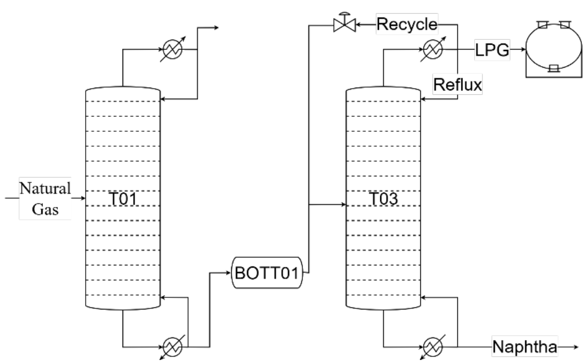



**Figure 6.** Simplified scheme of the NGPU used.

The control system was designed to have an optimization layer, given by the DMC3, and a regulatory layer, represented by different PI controllers present in the process. The main CVs of the process are:

- The ethane content of LPG
- The pentane content of LPG
- The Reid Vapor Pressure (RPV) of Naphtha
- The valve opening of the recycled flow rate of LPG back to the feed flow of the debutanizer column
- The condenser duty at the top of the debutanizer column
- The temperature at the top of the debutanizer column

The MVs for MPC are the setpoints of the variables:

- The reflux flow rate
- The temperature at the bottom of the demethanizer (T01)
- The temperature of the sensitive tray in the debutanizer (T03)
- The recycle flow rate
- The pressure at the top of the debutanizer
- The pressure at the bottom of the demethanizer

The simulation did not consider the presence of measurement noise. All variables were measured every minute without dead time. However, an artificial random noise was added to each sample of each variable to improve generalization.

### Data Generation

The simulation for generating the data was carried out considering 13 different scenarios with 10, 000 samples each. The scenarios include:

1. **Normal conditions:** absence of faults.
2. **Unmeasured disturbance:** a different disturbance applied to the system.
3. **Condenser loss of efficiency:** loss of efficiency in the condenser of the debutanizer column.
4. **Reboiler loss of efficiency:** loss of efficiency in the reboiler at the bottom of the demethanizer column.
5. **Valve stiction:** a dead band was considered in the recycled flow of LPG.
6. **Pentane content measurement error:** an offset in the measurement of pentane content was implemented.
7. **Recycle flow rate measurement error:** an offset in the measurement of recycled flow was implemented.
8. **Change in the PI tuning at the demethanizer column:** changes in the control tuning of the pressure controller.
9. **Change in the PI tuning at the debutanizer column:** changes in the control tuning of the recycle controller.
10. **Change in the MPC weights:** the weights related to the pentane content were modified to decrease the concern regarding this variable.
11. **Change in the MPC move suppression:** more free and aggressive movement of both the recycled flow rate and the temperature of the

sensitive tray in the debutanizer was considered.b

12. **MPC internal curves removed:** the curves describing the relationship between the setpoint of the recycled flow rate and the pentane content, the RPV of Naphtha, and the temperature at the top of the debutanizer were removed to simulate a plant-model mismatch.

13. **Change in model coefficients:** the coefficients of the curve that describe the relationship between the pentane content and the temperature at the sensitive tray of the debutanizer were changed to simulate an outdated model.

## Machine learning algorithms

The original dataset for both case studies was split randomly into data for training, validation, and testing, in the proportions of 64%, 16%, and 20%, respectively.

The input features for ML models, selected based on the physical knowledge of the system, were: the MVs included with up to two time lags; the integral of the time-weighted absolute errors (ITAE), considering the last 5 points of the controlled variables (CVs) with respect to their setpoints, and the prediction errors of these controlled variables. The ITAE of each CV was chosen to capture the error persistence through time, while the lagged MVs were chosen to capture dynamic behavior and the control actions. The prediction error, on the other hand, was chosen to capture model changes and the bias between the prediction and the measurement. This approach leads to a total of 10 features for the van de Vusse case study and 30 features for the debutanizer column.

RF and MLP were used to evaluate their performance in monitoring the NMPC and MPC closed loops. The implementations were carried out in Python. The architecture of each one was obtained by Optuna [20] after 100 trials, with the search conducted as follows:

- RF: The Python function RandomForestClassifier, from Scikit-learn, was used. Cross-validation was performed during optimizations, considering stratified K-folds with 5 folds. The objective function was the average accuracy of the test dataset. The optimized hyperparameters were:
  - Number of estimators between 10 and 100;
  - Maximum depth between 5 and 15;
  - Maximum features among "none", "sqrt", and "log2";
  - Minimum samples at each leaf between 5 and 10;
  - Criterion among "gini", "entropy", and "log_loss".
- MLP: The Python Tensor-Flow library was used. Early Stopping with a patience of 100 and a restore of the best weights was also used, considering the validation accuracy as a parameter. The reduction of the learning rate when accuracy achieved a plateau was also considered. The optimizer considered was Adam, and the batch size was 64. In each layer, a $L_2$ regularizer of 0.0001 was also used. The hyperparameters optimized were:
  - Number of layers between 2 and 4;
  - Number of neurons at each layer between 8 and 64;
  - Activation function among ReLU, LeakyReLU, and ELU;
  - Learning rate between $10^{-4}$ and $10^{-2}$;
  - Batch normalization between each layer: yes or no;
  - Dropout rate between 0.1 and 0.3.

F1-score and Accuracy, Equations (3) and (4), were used to compare RF and MLP results. TP denotes true positives, FP represents false positives, TN indicates true negatives, and FN refers to false negatives. An ideal scenario is one in which FP and FN are rare, while TP and TN are the majority. In such cases, these metrics tend to approach 1.

$$Accuracy = \frac{TP+TN}{TP+TN+FP+FN} \tag{3}$$

$$F1\text{-}score = \frac{2\times TP}{2\times TP+FP+FN} \tag{4}$$

The F1-score average used in this work, for both CMLM and SMLM, is the macro average, which calculates the F1-score for each label and then takes their unweighted mean. This average was used because, in this work, all classes are equally important, so they all have the same weight in the final value. Usually, on imbalanced datasets, the high metric score might be due to the correct classification of the majority class, while the minority class might have a poor result. The use of the unweighted average avoids this misinterpretation.

A total of 10 independent training sessions were performed for each ML model.

# RESULTS

Table 1 presents the metrics obtained for the multiclass classification and for each ML model of the CMLM for the Vande Vusse case study. The best results in Table 1, when comparing RF and MLP, are in bold font. It is possible to observe that models specializing in each fault have generally better performance than just a multiclass ML model. Only the first model, responsible for detecting abnormalities, when using MLP, has a slightly lower F1-score. The low standard deviation observed in each model training indicates that the metric values are consistent over the 10 independently trained models.

**Table 1:** Metrics of each ML model for the van de Vusse case study.

| ML | RF | | MLP | |
|---|---|---|---|---|
| Metric | Accuracy | F1 score | Accuracy | F1 Score |
| Multiclass | 0.8087 ± 0.0037 | 0.8128 ± 0.0038 | **0.8491 ± 0.0367** | **0.8502 ± 0.0397** |
| M1: Detection | 0.8379 ± 0.0023 | **0.8351 ± 0.0024** | **0.8789 ± 0.0047** | 0.8073 ± 0.0108 |
| M2: Valve Stiction | 0.9104 ± 0.0029 | 0.8885 ± 0.0038 | **0.9442 ± 0.0059** | **0.9244 ± 0.0078** |
| M3: Tuning | 0.9772 ± 0.0020 | 0.9746 ± 0.0022 | **0.9918 ± 0.0026** | **0.9908 ± 0.0029** |
| M4: Mismatch | **0.9679 ± 0.0019** | **0.9679 ± 0.0019** | 0.9580 ± 0.0025 | 0.9579 ± 0.0025 |

Before analyzing the results, it is important to understand how Accuracy and F1-score values should be compared. Accuracy is less sensitive to imbalanced datasets, and its high value might be due to the excellent performance of the majority class, independently of the minority class results. However, since the F1-score is taking the macro average, this metric is fairer to take into consideration the minority class, as all labels are treated as equally important. In M4 (diagnosing mismatch), where data is perfectly balanced, both the F1-score and Accuracy have similar values. M1 (detection), on the other hand, has a discrepancy between the values of those two metrics, which might be due to the artificial imbalance created in the cascade. Once the problem is turned into a binary classification, normal data becomes the minority class when compared to the other labels for this model. For this reason, F1-score is used as the priority metric to compare MLP and RF, while Accuracy is used to evaluate how well the majority class is being classified.

By comparing the performance of RF and MLP for each diagnostic model, it is possible to observe that RF models were better in diagnosing the parameter of mismatch (M4), while MLP models had slightly better performance in diagnosing valve stiction and poor tuning (M2 and M3). In the first model, responsible for detecting abnormalities in the control loop, the performance of MLP was better in terms of accuracy. However, the F1-score shows that this first model has better results with RF.

The reason for RF having better results in some situations might be due to the nature of this algorithm. RF based its predictions on hard boundaries of each feature, while MLPs are better at capturing nonlinear relationships between variables. For detection (M1) and diagnosis of mismatch (M4), the diagnosis is more based on whether the variables are higher than a given value. For the diagnosis of valve stiction (M2) and poor tuning (M3), which both cause oscillation in the closed-loop, MLP might be better suited to capture this nonlinear interaction.

The main advantage of using CMLM is that it gives a prompt diagnosis without exhaustive data investigation. One of the traditional methodologies applied in industry is using the standard deviation of variables to capture variability changes. This analysis is based on the minimum variance control theory and on the Harris Index [21] to monitor control performance. Aspen Watch and Schneider Electric's EcoStruxure Control Expert also use the variables' standard deviation as one of the metrics to evaluate the closed loop. Figure 7 shows the standard deviation time history of each MV ($F/V$ and $\dot{Q}$) and CV ($C_B$ and $T$) using a moving window of 100 samples (15 min of simulation). Visually, both the normal (blue area) and the valve stiction (green area) have the same range of standard deviation values, except for some samples equal to 0 for the $F/V$. Changes in the NMPC tuning and in its internal model parameters cause the standard deviation range for some variables to be different than those observed in normal conditions, especially regarding the tuning changes. However, the standard deviation gives information regarding a specific variable and does not give a clue to the root cause of this performance degradation.

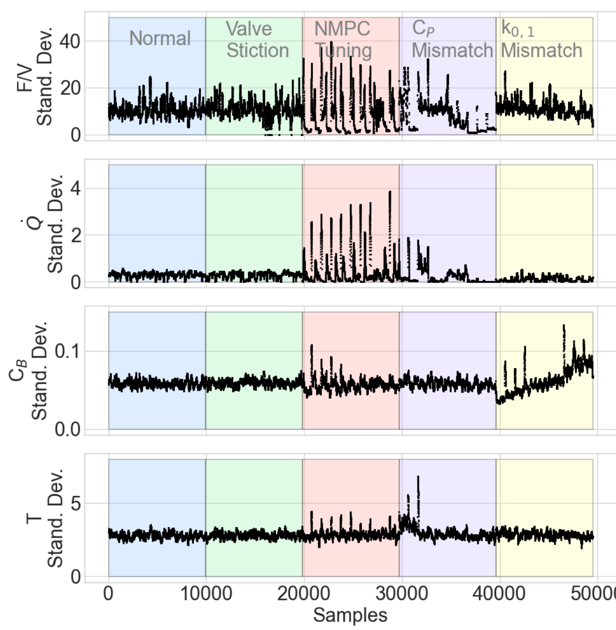



**Figure 7.** Standard deviation of the van de Vusse reactor.

To evaluate the method's scalability for industrial MPC implementations, a similar approach was tested in a debutanizer column. The results obtained are in Table 2, considering the cascade presented in Figure 3. The low standard deviation indicates the stability of the results. The metric values show that most of the models in the

**Table 2:** Metrics of each ML model for the debutanizer column case study.

| ML | RF | | MLP | |
|---|---|---|---|---|
| Metric | Accuracy | F1-score | Accuracy | F1-score |
| Multiclass | 0.9350 ± 0.0013 | 0.8972 ± 0.0016 | 0.9479 ± 0.0006 | 0.9151 ± 0.0031 |
| M1: Detection | 0.9239 ± 0.0041 | 0.7554 ± 0.0079 | **0.9977 ± 0.0003** | **0.9871 ± 0.0017** |
| M2: Process or controller | 0.9407 ± 0.0011 | 0.9393 ± 0.0012 | **0.9487 ± 0.0010** | **0.9466 ± 0.0015** |
| M3: Disturbance | 0.9983 ± 0.0003 | 0.9945 ± 0.0009 | **0.9998 ± 0.0001** | **0.9995 ± 0.0002** |
| M4: Equipment or Instrumentation | 0.9996 ± 0.0001 | 0.9996 ± 0.0001 | **0.9999 ± 0.0001** | **0.9999 ± 0.0001** |
| M5: Which equipment | **0.9999 ± 0.0001** | **0.9999 ± 0.0001** | 0.9999 ± 0.0001 | 0.9999 ± 0.0001 |
| M6: Valve or sensors | 0.9987 ± 0.0003 | 0.9985 ± 0.0003 | **0.9995 ± 0.0002** | **0.9995 ± 0.0002** |
| M7: Which sensor | **0.9999 ± 0.0001** | **0.9999 ± 0.0001** | 0.9999 ± 0.0001 | 0.9999 ± 0.0001 |
| M8: MPC or PI | 0.9995 ± 0.0002 | 0.9993 ± 0.0003 | **0.9998 ± 0.0002** | **0.9997 ± 0.0002** |
| M9: Which PI | **0.9950 ± 0.0010** | **0.9950 ± 0.0010** | 0.9950 ± 0.0003 | 0.9721 ± 0.0018 |
| M10: MPC tuning or model | 0.9956 ± 0.0007 | 0.9956 ± 0.0007 | **0.9985 ± 0.0005** | **0.9985 ± 0.0005** |
| M11: Which tuning parameter | 0.9954 ± 0.0006 | 0.9954 ± 0.0006 | **0.9989 ± 0.0004** | **0.9989 ± 0.0004** |
| M12: Which model issue | 0.9997 ± 0.0002 | 0.9996 ± 0.0002 | **0.9998 ± 0.0002** | **0.9998 ± 0.0003** |

CMLM approach have a better performance than the SMLM. Only the RF M1, responsible for the detection, has significantly lower performance. This may have occurred because the RF algorithm cannot capture the more complex differences between normal and abnormal samples using thresholds.

By comparing the performance between RF and MLP models, the MLP models outperformed RF in most models of the CMLM, even though some of them have just a slight difference. Curiously, the RF models in the CMLM that have a similar or better performance than the MLP models are those responsible for diagnosing between two alternatives of the same type of equipment (M5: which process equipment, M7: which sensor, M9: which PI). This might have happened due to the characteristic of the RF algorithm, which is better suited to classify problems related to a given threshold. Since those alternatives affect different variables in the process, RF can handle the classification properly.

Regarding the computational cost, for the evaluation of 1, 000 random samples for the debutanizer column, the CMLM spends an average of 0.4 seconds per sample for the MLP, with a maximum time of 1.4 seconds. This was evaluated on a computer with Intel(R) Core (TM) i7-12700, CPU 2.10 GHz, and 16.0 GB of RAM. This evidence reinforces the capability of CMLM to be applied to online monitoring.

## CONCLUSIONS

One of the goals of this study is to highlight the potential of using ML models for monitoring and diagnosing MPC performance. The method is more accurate than those currently used in industrial applications. The results show that ML models have the potential to diagnose control performance issues precisely, with CMLM having superior performance to a single multiclass model approach by isolating fault characteristics. By combining independent ML models, it is possible to use different model structures than a single type of ML model, taking advantage of the strengths of each ML tool. The two case studies show that the methodology can be implemented in both small and large industrial MPC applications. Even though the plant-model mismatch classification is too narrow and the source is usually not known, the case studies assume that the source of MPC degradation was limited to a few possibilities to explore how accurate the diagnosis of the ML models is. The diagnosis might be adapted to require the identification of only part of the process, instead of requiring the reidentification of the whole plant.

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## AUTHOR IDENTIFIERS

Author ORCIDs:
Melo EV: 0009-0006-5566-8413
Secchi AR: 0000-0001-7297-3571
Souza MB Jr: 0000-0002-1090-8958

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