MULTIVARIATE PROCESS MONITORING

Fault Detection, Diagnosis, and Prognosis using PCA, Takens-PCA, CVA, and CVDA

Data Mining & Wrangling 1 Final Project
MSDS 2026 | November 24, 2025

9
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Toxic gas leak at Indian chemical plant kills at least 11 and hospitalizes hundreds

By Vedika Sud, Akanksha Sharma, Jessie Yeung, Esha Mitra and Emma Reynolds, CNN
6 min read · Updated 3:47 PM EDT, Thu May 7, 2020

1 dead, 76 hospitalized due to ammonia leak in Navotas

By Joyce Ann L. Rocamora
February 3, 2021, 9:06 pm

Share

BAY AREA

'Series of safety failures' led to devastating Martinez refinery fire that burned worker

By **Molly Burke**, Staff Writer
Updated March 14, 2025 6:35 p.m.

U.S. NEWS

Deadly chocolate factory explosion caused by faulty gas fitting, safety board finds

How can Data Science

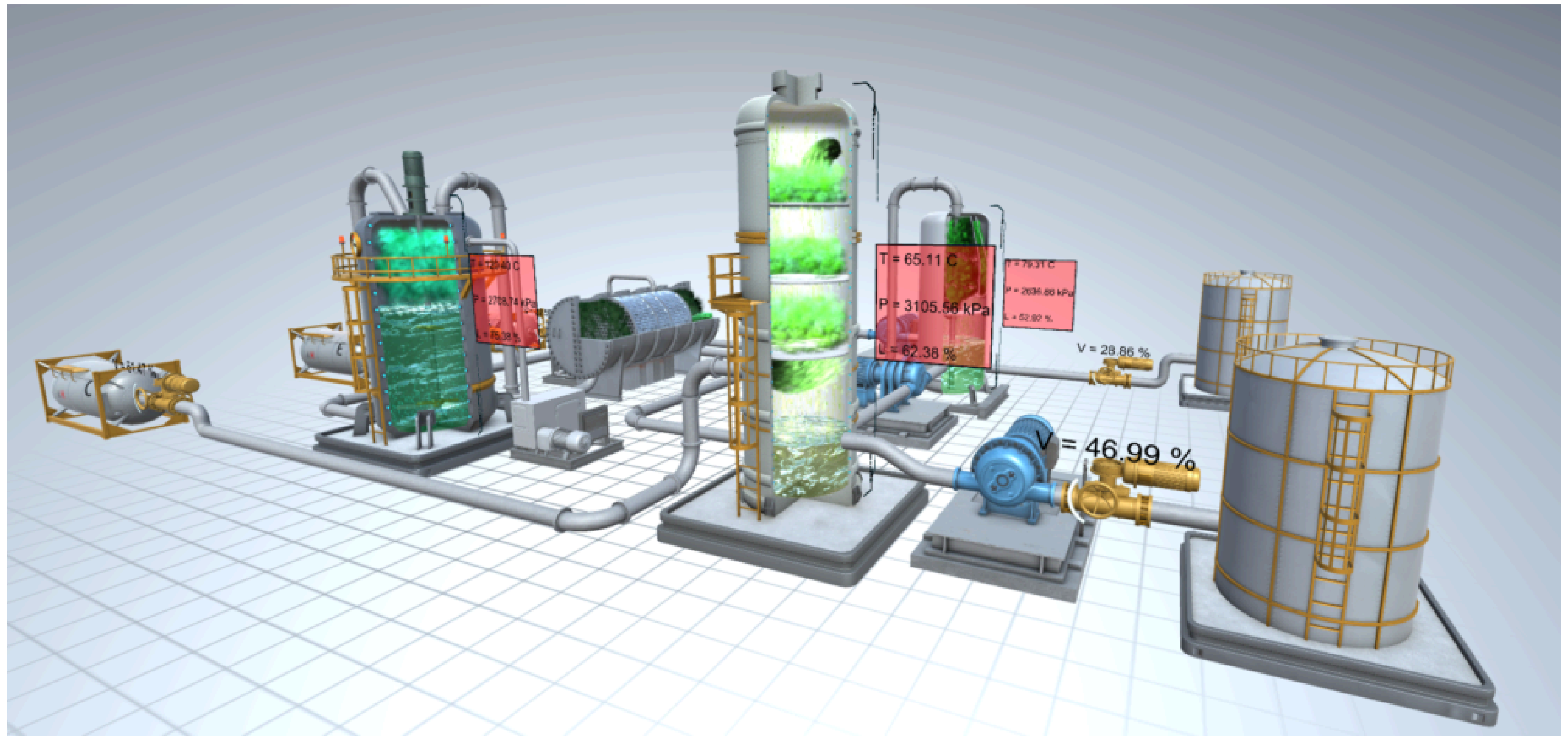
help prevent the next one?

OBJECTIVES

This study seeks to understand the health of an industrial process by addressing three fundamental questions:

FAULT DETECTION	Has a fault occured?
FAULT DIAGNOSIS	Where did it occur?
FAULT PROGNOSIS	How will it progress in the future?

DATA BACKGROUND



Tennessee Eastman Process
Dynamic Simulation Logs

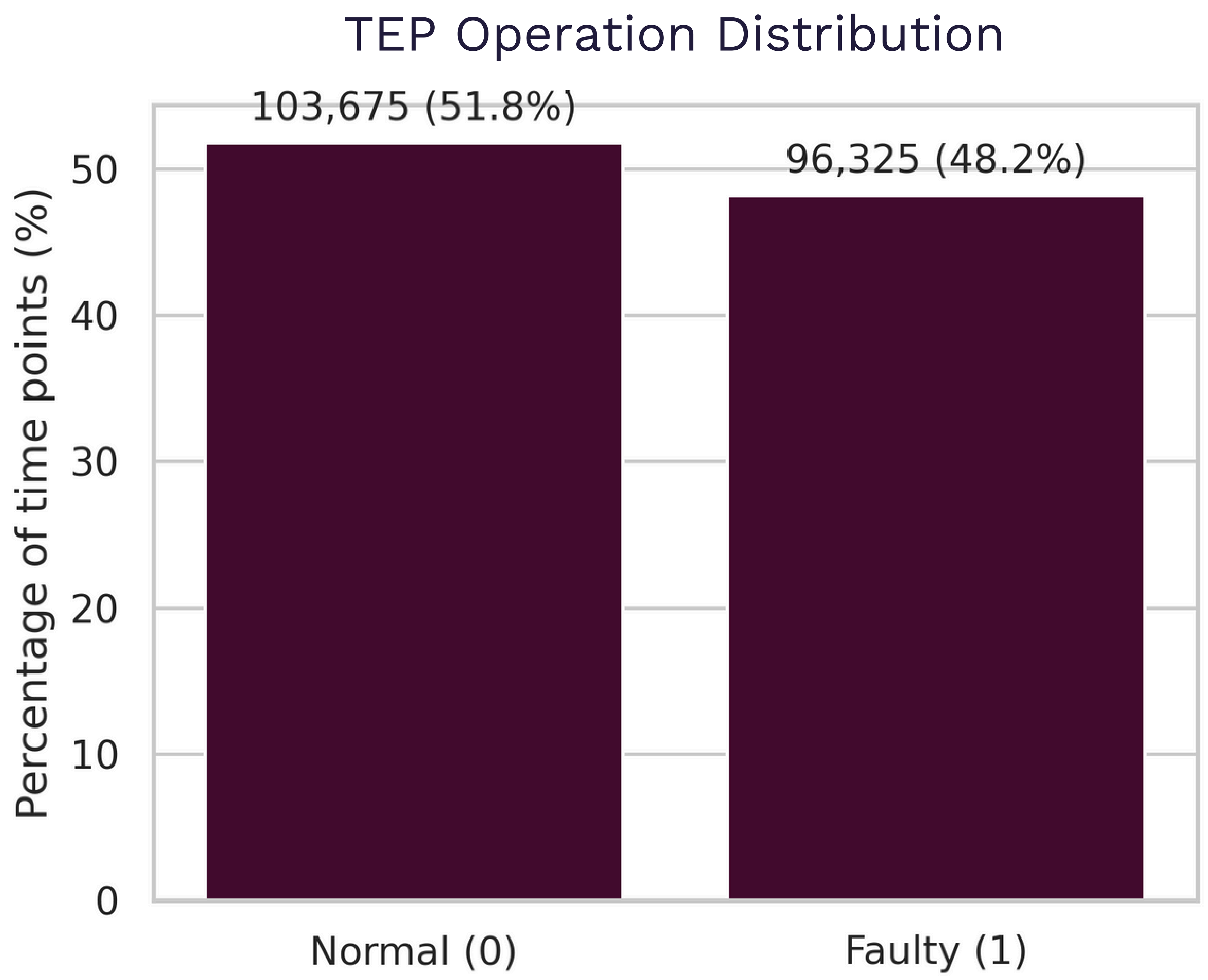
A large chemical plant running normally, with selected faults introduced during certain periods.

SPAN, SIZE, FREQUENCY
- 3 years (1970-1972)
- ~525k rows
- variables recorded every 3 mins

VARIABLES
All variables are real plant sensor readings
- 41 process measurements (XMEAS)
- 12 manipulated variables (XMV)
- 1 status code (0 - normal operating condition)

ZERO MISSING VALUES
ZERO DUPLICATES

NORMAL VS FAULTY



TEP shows Balanced Mix
52% Normal, 48% Faulty

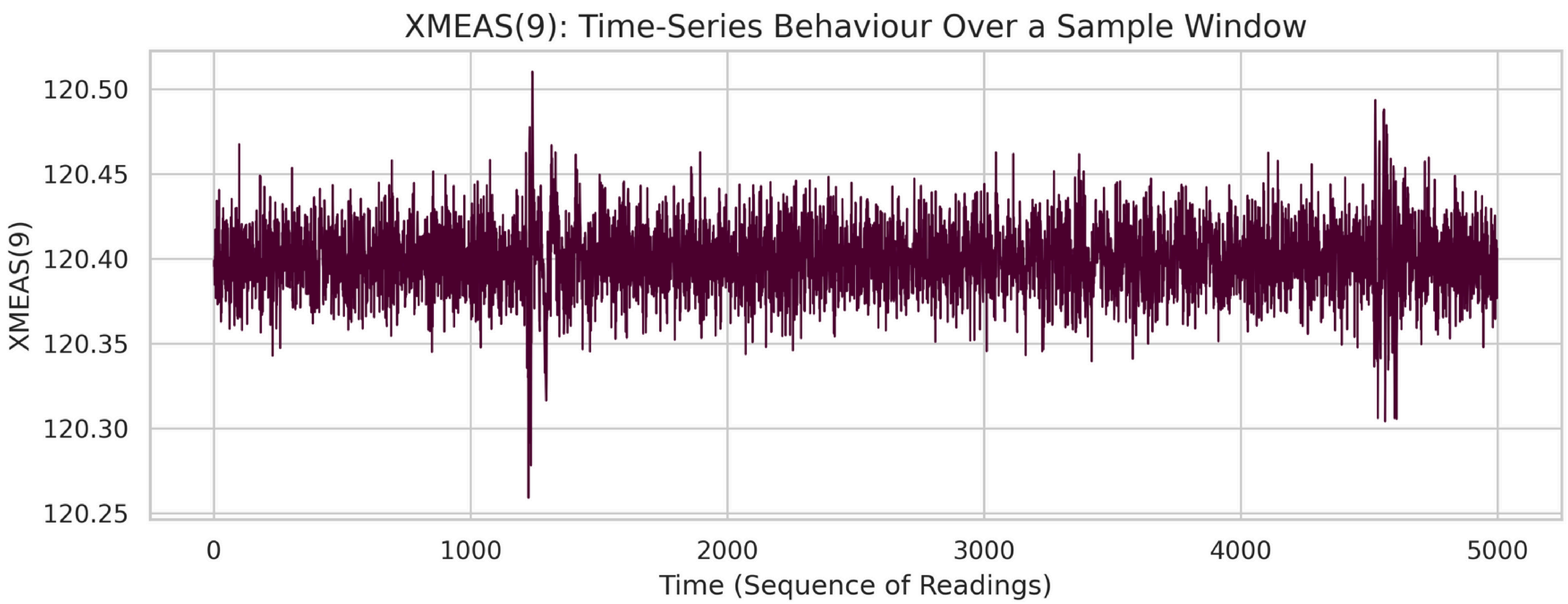
WHAT IS A FAULT?
In industrial processes like TEP, a fault means something in the system is *no longer behaving normally.*

- Abrupt fault
  something breaks suddenly

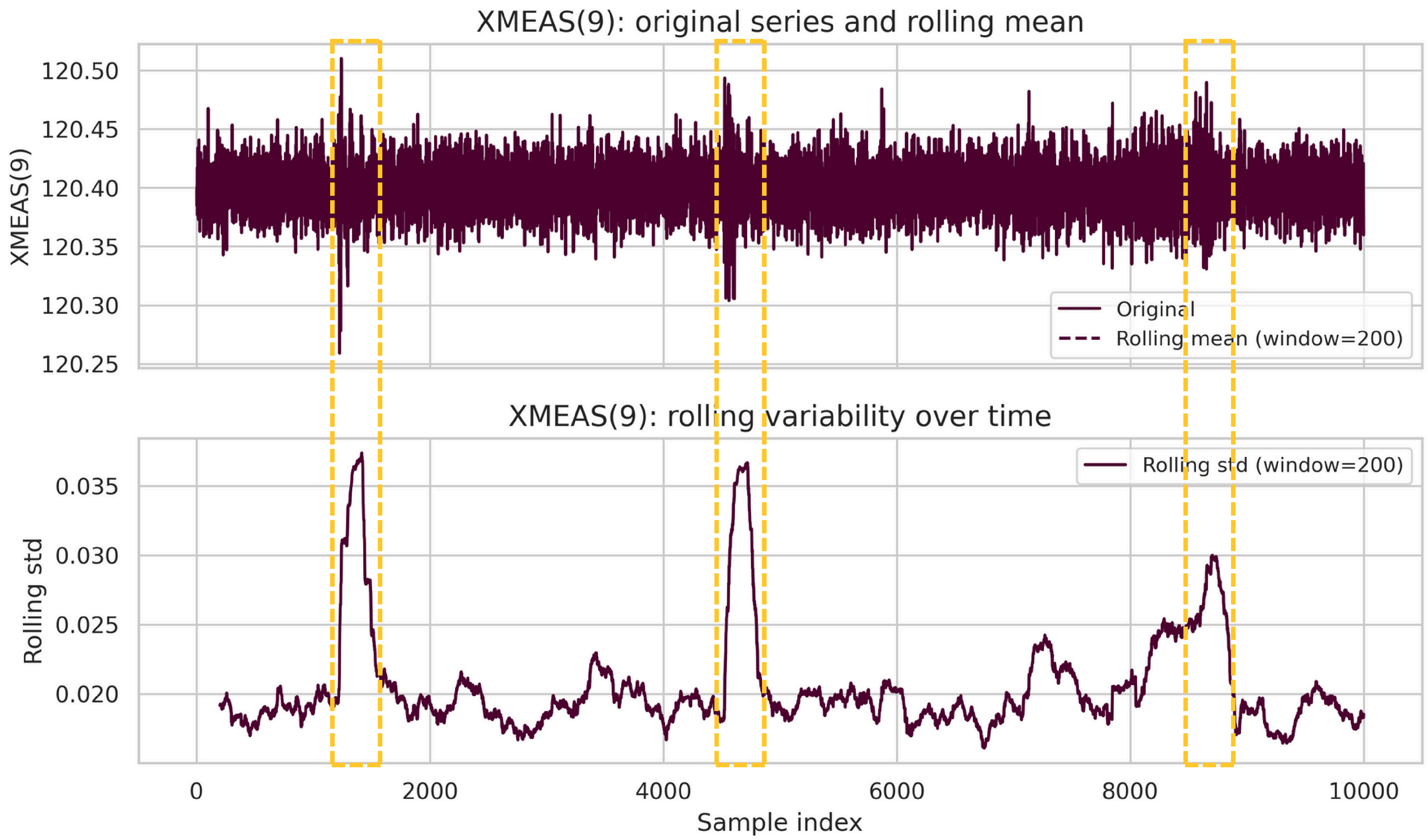
- Incipient fault
  something slowly degrades over time

TIME-SERIES NATURE

SAMPLE CASE: **XMEAS(9) - Reactor Temperature**

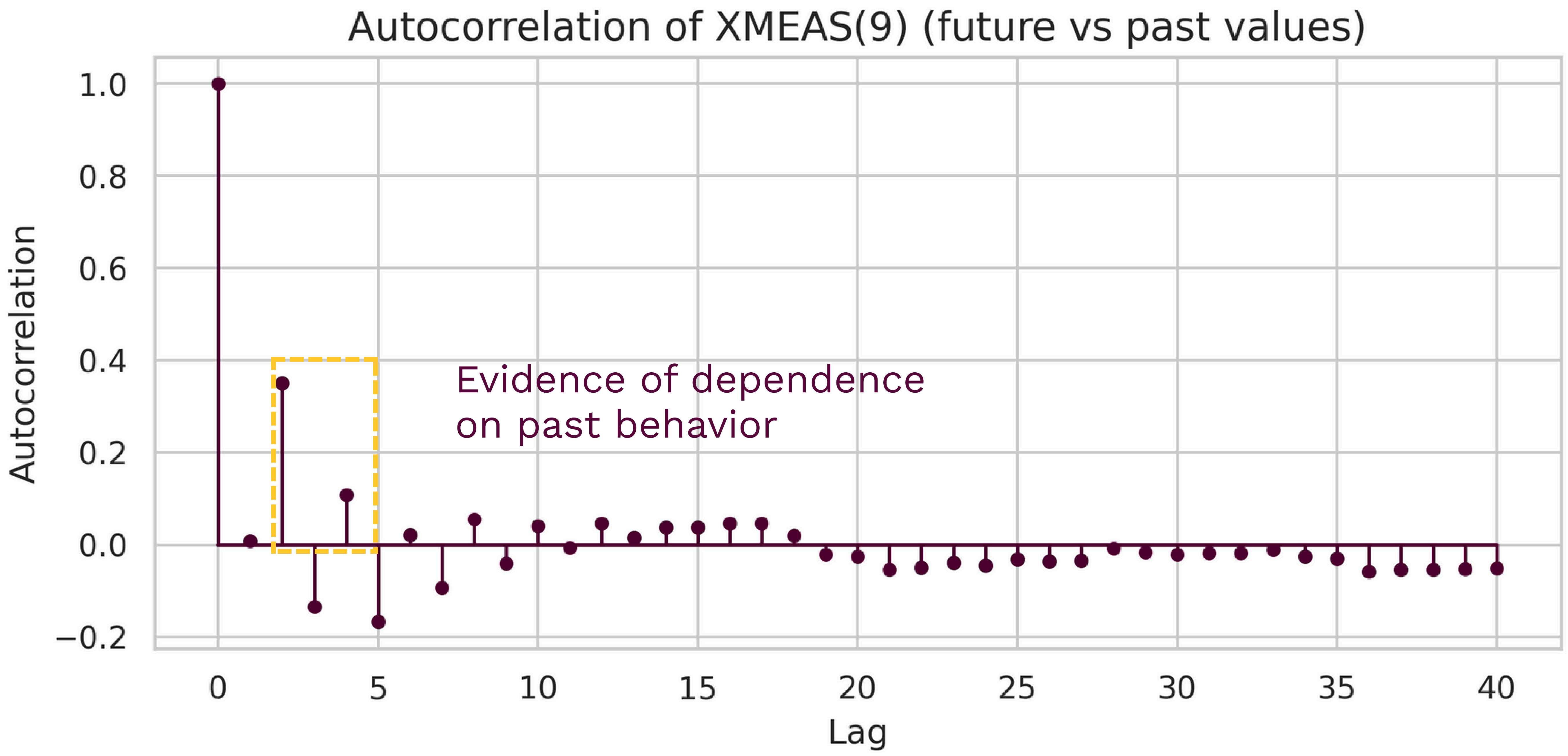


Reactor temperature shows small, steady fluctuations within a narrow band, indicating stable and controlled operation.



At certain points, variability suddenly increases. The readings start to spread out, indicating reduced stability. These shifts can be early warning signs before a fault appears.

TIME-SERIES NATURE



The temperature doesn't move randomly — each reading follows the one before it. The tall bars show strong memory of recent values, while the small dips below zero show the control system making tiny corrections.

How do we proceed

when the variables are time-series?

THEORETICAL FRAMEWORK

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THEORETICAL FRAMEWORK

FAULT DETECTION

70-30 Train-Test Split

Train (Normal)	(185438, 52)	Model learns normal behavior
Test (Normal)	(79474, 52)	Can the model stay quiet when nothing is wrong?
Test (Faulty)	(260688, 52)	Can the model alarm when something is wrong?

BASELINE

INPUT → STATIC PCA → OUTPUT

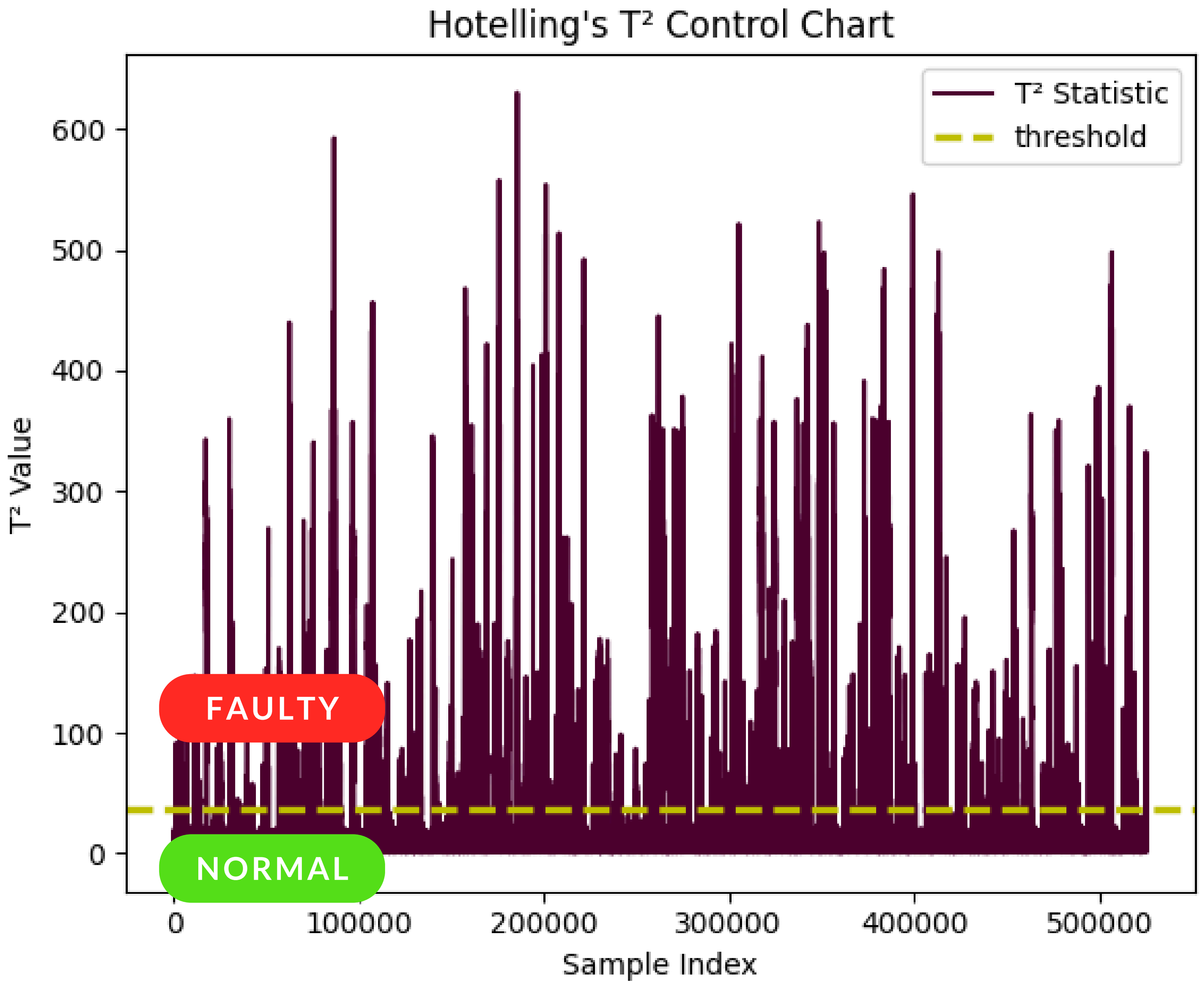
INPUT
Test Set
(Normal + Faulty)

STATIC PCA
Trained on Normal Operations

OUTPUT
- Alarm Trigger (Yes/No)
- Detection Delay
- Detection Rate (DR)

THEORETICAL FRAMEWORK

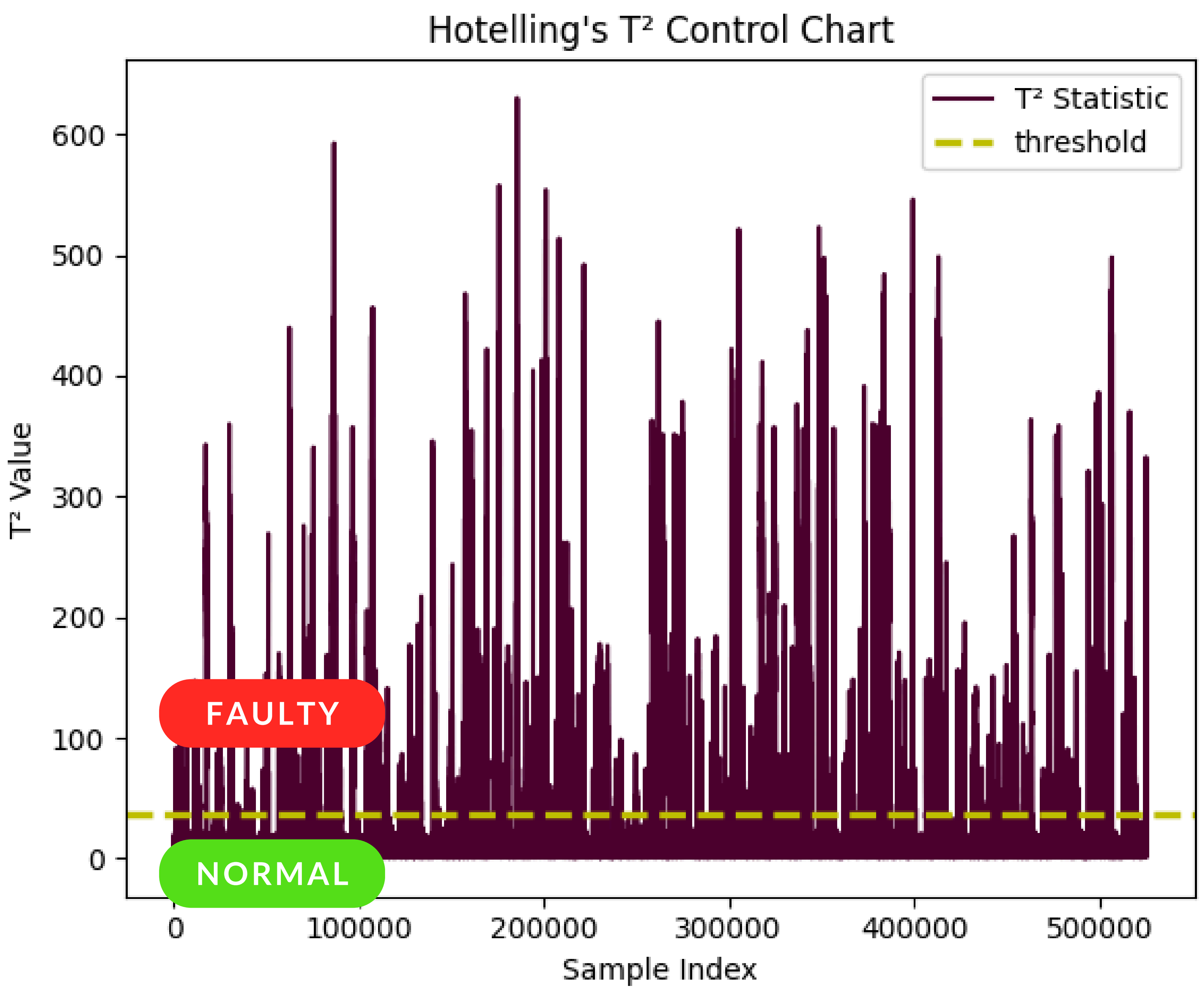
FAULT DETECTION

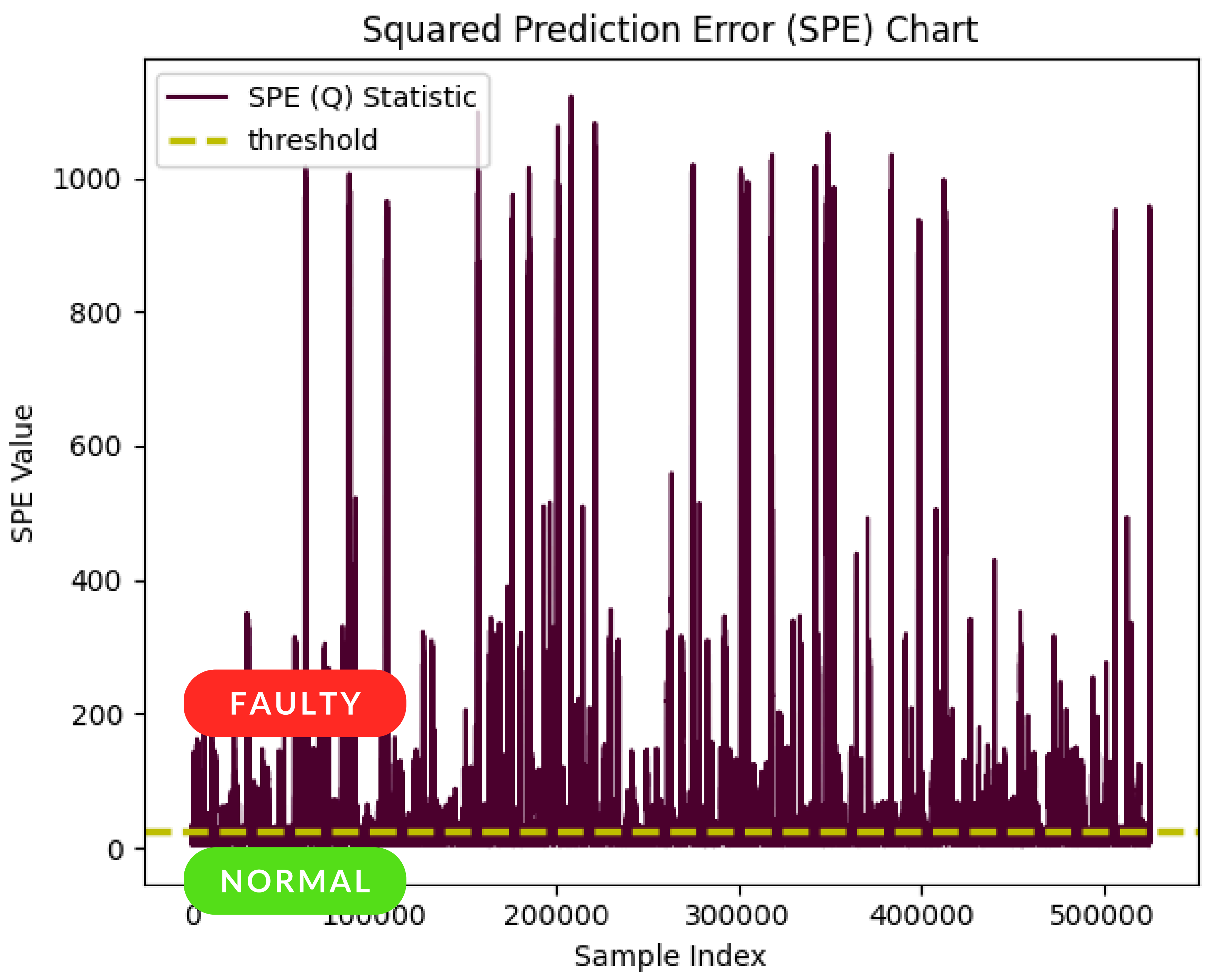


Statistic	How it Detects?	Best For
T^2	Flags large shifts inside the PCA model	Abrupt faults
Q / SPE	Flags unexplained behavior outside the PCA model	Incipient faults

THEORETICAL FRAMEWORK

FAULT DETECTION





THEORETICAL FRAMEWORK

FAULT DETECTION

Detection Methods

Static PCA (*Baseline*)	*Principal Component Analysis (PCA)*	Detects deviations from normal patterns using T^2 and Q limits.
Dynamic PCA	*Takens-PCA*	Adds time memory to PCA for better drift and trend detection.
CVA	*Canonical Variate Analysis (CVA)*	Detects faults by comparing predicted vs. actual system behavior.
CVDA	*Canonical Variate Dissimilarity Analysis (CVDA)*	Uses a dissimilarity index (D-index) for highly sensitive detection, especially for incipient faults.

THEORETICAL FRAMEWORK

FAULT DETECTION | FAULT DIAGNOSIS | FAULT PROGNOSIS

STEP 1
Detect Abnormality
Use T^2, Q/SPE, and D-index charts to confirm that a fault has occurred.

STEP 2
Model Behavior
Apply PCA, DPCA, CVA, and CVDA to capture correlations and dynamics.

STEP 3
Variable Contributions
Identify which variables drive the T^2, Q, or D-index exceedances.

STEP 4
Locate Fault
Map contributing variables to process units (reactor, stripper, separator, etc.)

STEP 5
Assess over Time
Check if contributions are stable, growing, or fluctuating to understand if the fault is abrupt or progressing.

RESULTS & DISCUSSIONS

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REAL TIME DETECTION

FAULT DETECTION

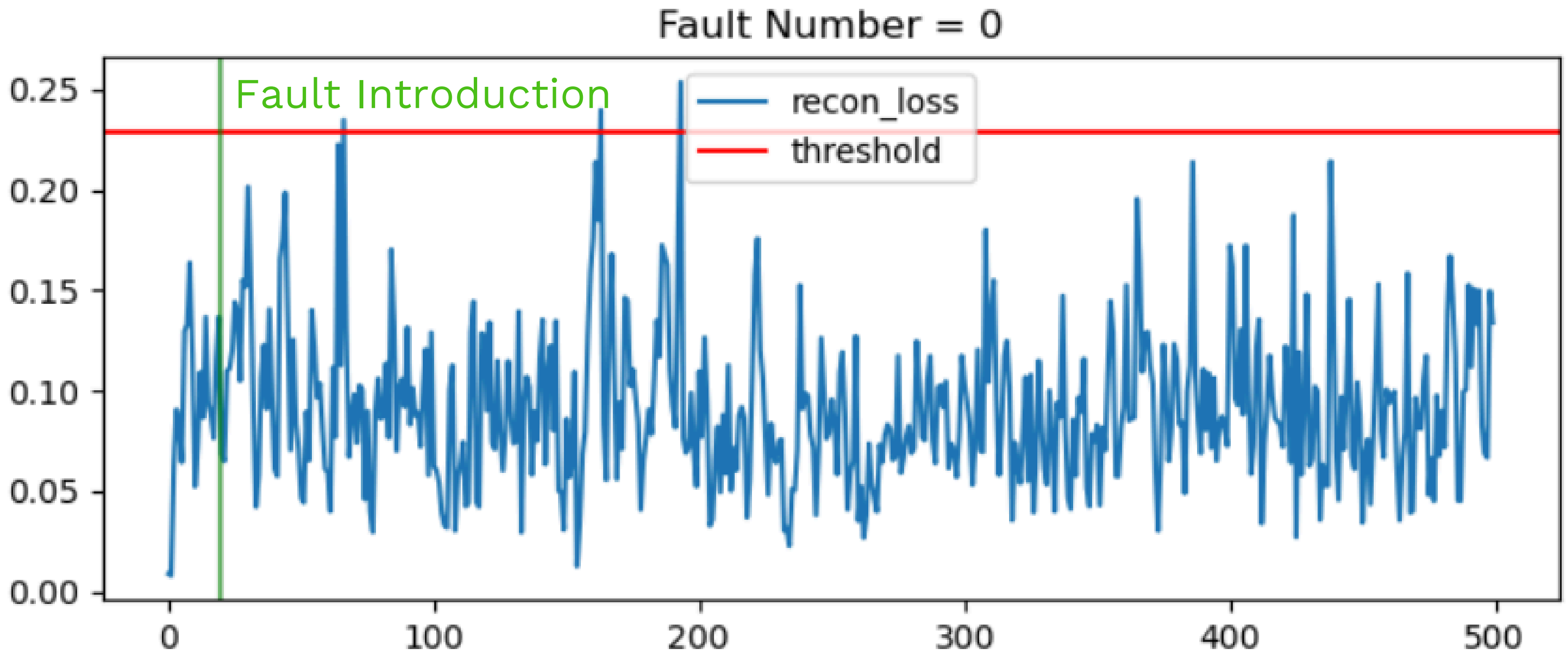
BASELINE

INPUT → **STATIC PCA** → **OUTPUT**

INPUT: Test Set (Normal + Faulty)

STATIC PCA: Trained on Normal Operations

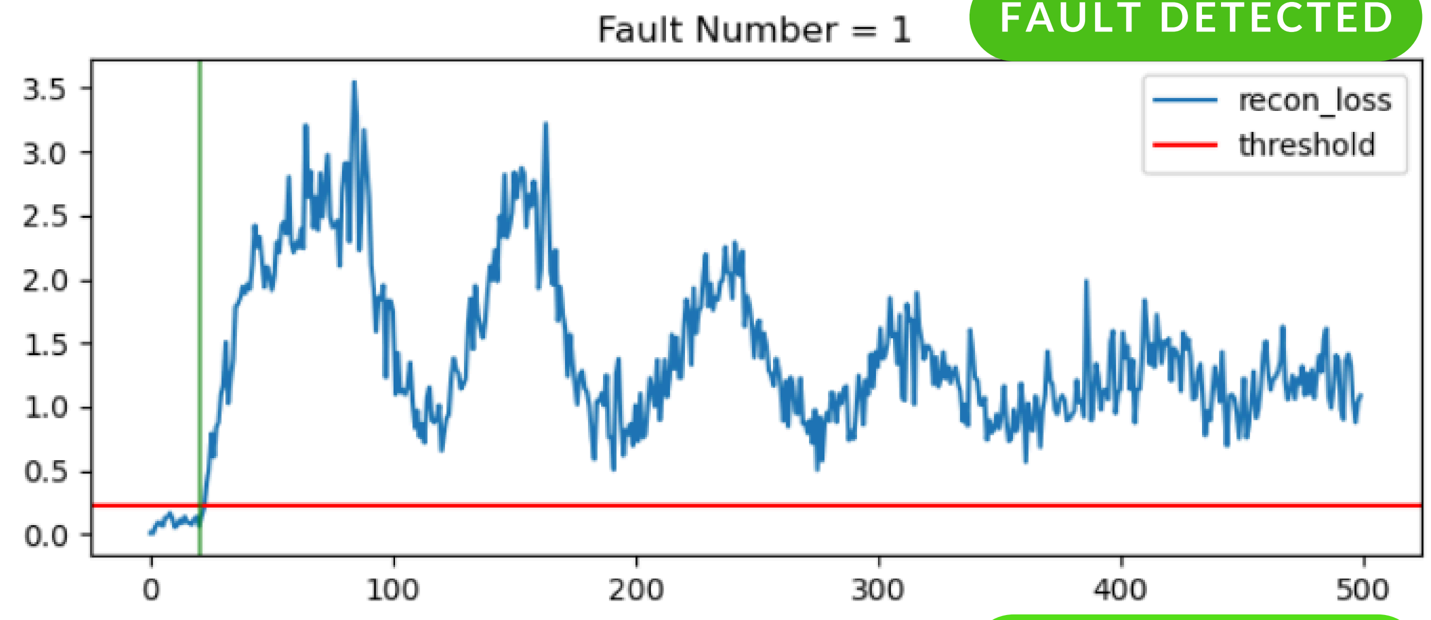
OUTPUT:
- Alarm Trigger (Yes/No)
- Detection Delay
- Detection Rate (DR)



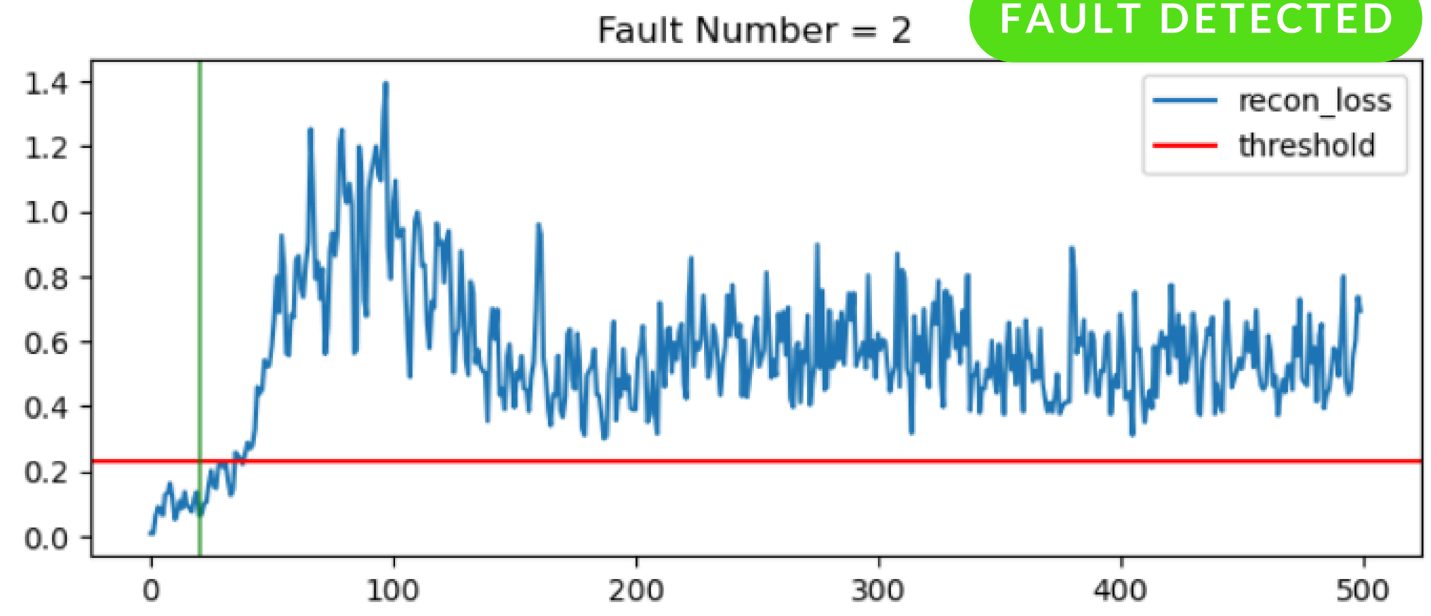
Threshold = Normal Operation Reconstruction Loss

Reconstruction loss is the error resulting from the difference between the original data and its reconstructed version after dimensionality reduction (like PCA)

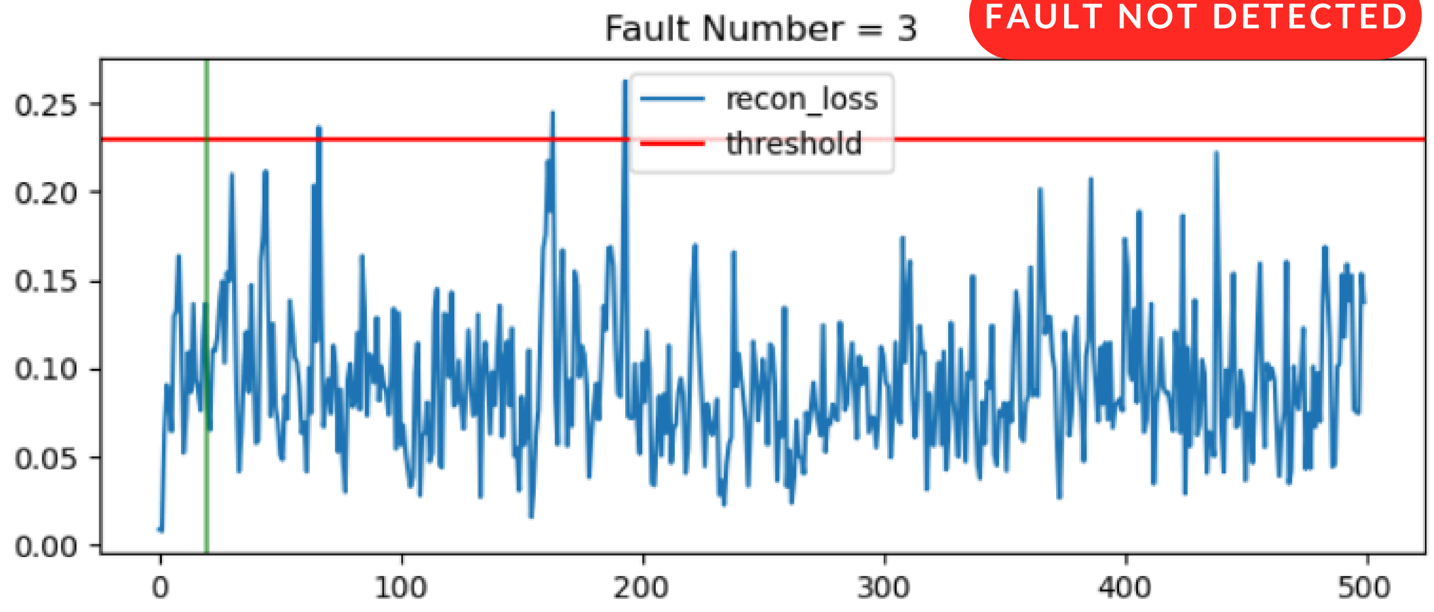
FAULT DETECTED



FAULT DETECTED



FAULT NOT DETECTED



DETECTION SUMMARY

FAULT DETECTION

Method	Average Detection Rate
Dynamic PCA	39.10%
Static PCA	26.00%
CVA	24.70%
CVDA	13.50%

Takens-PCA (DPCA)
Best Average DR

52 variables → 156 variables with lag
46 kept (90.26% variance explained)

Fault Category	Fault Numbers	Average Detection Rate
Process Faults	F1 - F9	66.20%
Mechanical Faults	F10 - F15	37.20%
Stochastic Faults	F16 - F20	20.70%

Process Faults
Most Detectable

DETECTION SUMMARY

FAULT DETECTION

Rank	Fault No.	Fault Definition	Best DR	Best Method
1	F4	Step Feed E comp. (Process)	100.00%	DPCA (Q)
2	F6	Feed B temp var. (Process)	100.00%	DPCA (Q)
3	F7	Feed C temp var. (Process)	99.80%	DPCA (T2)
4	F5	Feed A temp var. (Process)	98.40%	CVA (Q)
5	F1	Step A/C ratio (Process)	97.10%	PCA (Q)
6	F2	Step Feed B comp. (Process)	94.30%	DPCA (T2)
7	F14	Separator valve stuck (Mechanical)	74.90%	DPCA (T2)
8	F11	Condenser valve stuck (Mechanical)	60.20%	DPCA (Q)
9	F13	D feed valve stuck (Mechanical)	42.50%	PCA (Q)
10	F17	Condenser temp (Rand.) (Stochastic)	43.70%	PCA (Q)

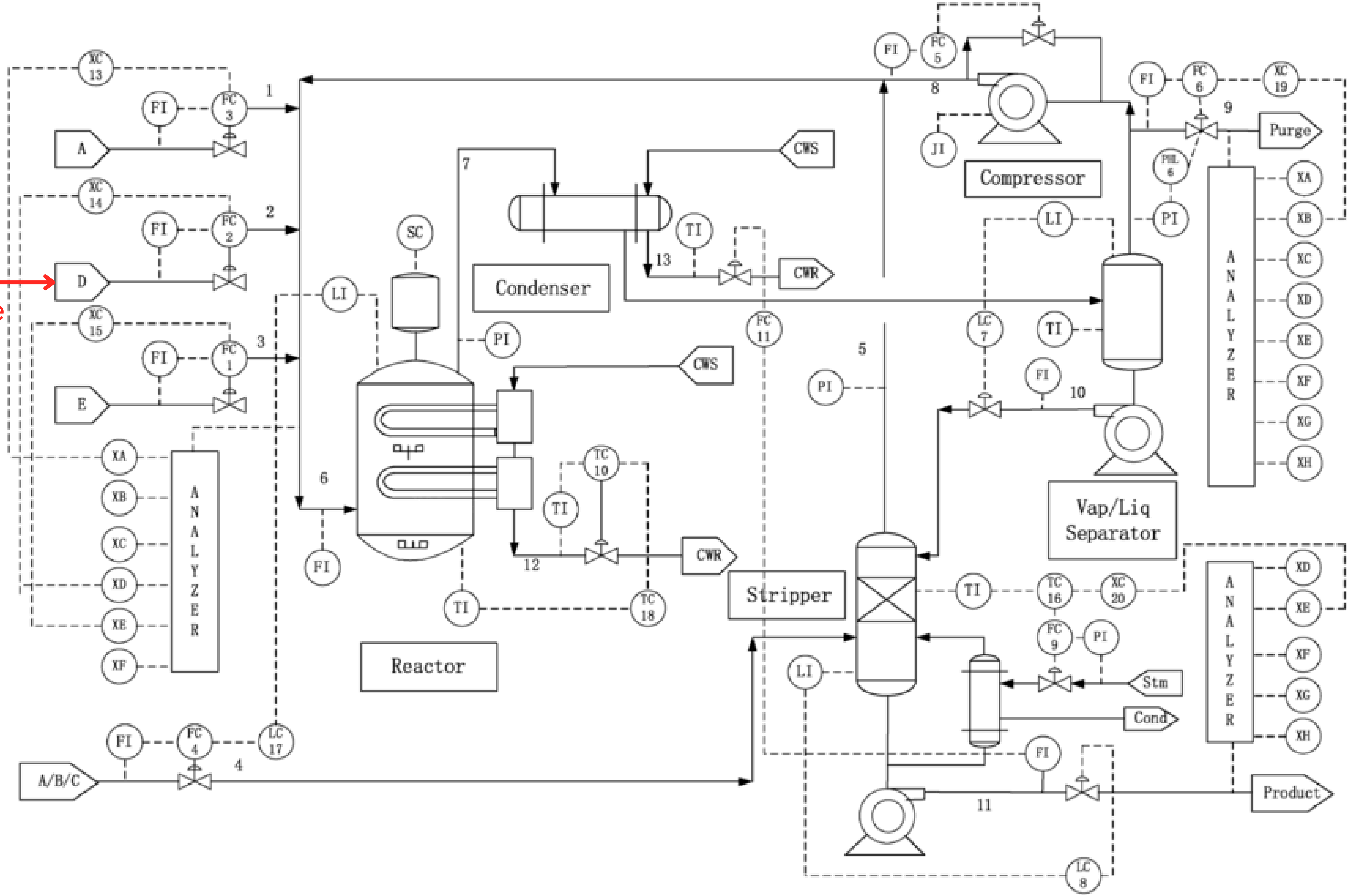
DETECTION SUMMARY

FAULT DETECTION

Rank	Fault No.	Fault Definition	Best DR	Best Method
11	F12	A feed valve stuck (Mechanical)	43.30%	DPCA (Q)
12	F16	Reactor temp (Rand.) (Stochastic)	24.20%	CVDA (D)
13	F20	Feed A temp (Rand.) (Stochastic)	23.90%	DPCA (Q)
14	F18	Feed A comp (Rand.) (Stochastic)	11.80%	CVA (Q)
15	F8	Feed D temp var. (Process)	4.80%	CVA (Q)
16	F10	Reactor valve stuck (Mechanical)	1.50%	CVDA (D)
17	F9	Condenser temp var. (Process)	0.70%	CVDA (D)
18	F15	Stripper valve stuck (Mechanical)	0.60%	CVDA (D)
19	F3	Step Feed D comp. (Process)	0.50%	CVDA (D)
20	F19	Feed B comp (Rand.) (Stochastic)	0.10%	DPCA (Q)

FAULT 2: SUDDEN INCREASE IN STREAM 2

Step Change of Feed in Stream 2



HAS FAULT 2 OCCURED?

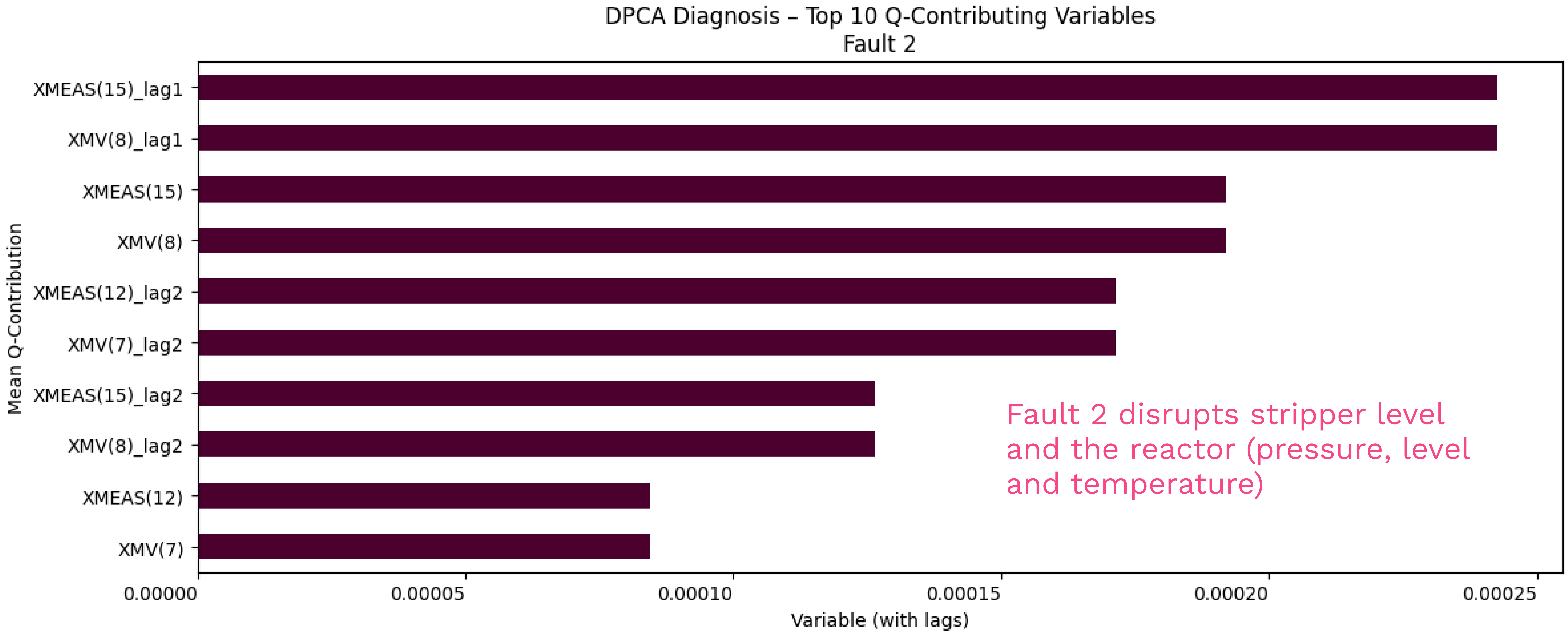
FAULT DETECTION YES. ITS DETECTED BY T^2.

Method	Metric	Detection Rate	Detection Delay	False Alarm Rate
PCA	T^2	93.90%	43	0.79%
DPCA	T^2	94.30%	41	0.99%
CVA	T^2	92.50%	50	1.00%
PCA	Q	1.20%	64	0.83%
DPCA	Q	0.77%	62	1.06%
CVA	Q	0.07%	16162	1.03%
CVDA	*D-index*	0.87%	824	1.00%

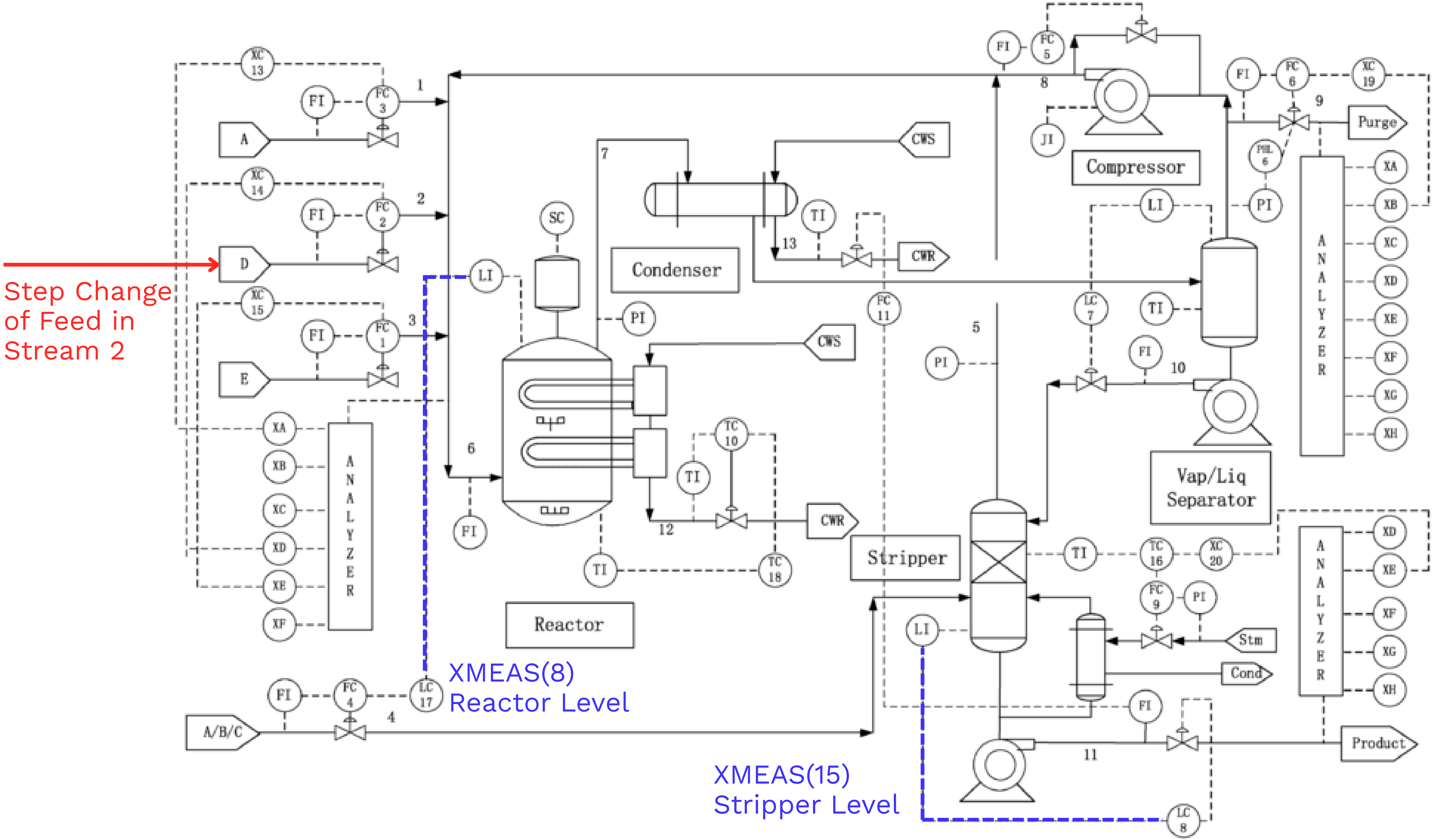
- Fault 2 is an abrupt fault → T^2 detects it strongly, but Q/D-index barely respond.
- DPCA-T^2 is the best detector → highest detection rate (94.3%) and fastest detection (41 samples ≈ 123 minutes).

WHERE DID IT OCCUR?

FAULT DIAGNOSIS IN THE STRIPPER AND REACTOR

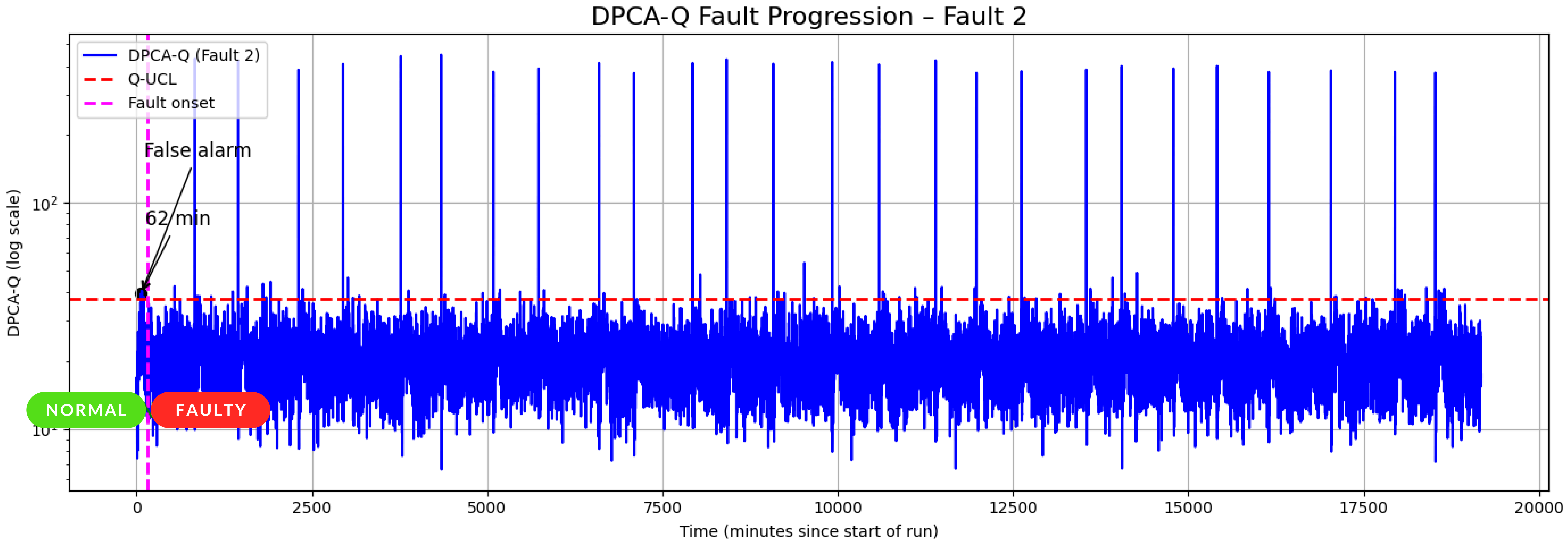


FAULT 2: SUDDEN INCREASE IN STREAM 2



HOW WILL IT PROGRESS?

FAULT PROGNOSIS IT DID NOT PROGRESS



Fault 2 did not evolve into a growing or worsening condition; it stays as a sudden, abrupt disturbance with no clear increase in severity over time.

IMPLICATIONS

Conclusion

- Fault 2 has been detected and it affected the stripper–reactor system.
- No progression over time, meaning the disturbance is there but likely controlled by Flow controls cascaded with Level Indicators and Controllers

Next Steps

- Apply the same *detect* → *diagnose* → *prognose* framework to all remaining faults given in the TEP dataset
- Build a fault behavior library to guide risk-based and prioritized interventions.
- Address high-risk or fast-progressing faults first, while stable faults can be planned.

Important Note

- Analysis is limited by dataset and domain knowledge.
- Final operational decisions must be validated by plant engineers and process experts.

FAULT BEHAVIOR LIBRARY

Fault No.	Fault Description	Top Contributing Variables	Implications
1	Feed A/C Ratio Change (Composition)	XMEAS(23), XMEAS(38) (Product Composition)	Product Purity is wrong. The final chemical mix is immediately different.
2	Feed B Composition Change	XMEAS(15), XMV(8) (Stripper Level/Flow)	The Stripper Level is unstable. The liquid separation unit goes haywire.
3	Feed D Composition Change	XMV(1), XMEAS(2) (D Feed Flow/Valve)	D Feed Valve is compensating hard. The controls are frantically adjusting D Feed flow to fix the mix.
4	Feed E Composition Change	XMV(10) (Reactor Cooling-Water Flow)	Reactor is too hot/cold. The main cooling valve has to slam open or shut due to the heat change.
5	Feed A Temperature Variation	XMV(11) (Condenser Cooling-Water Flow)	Condenser is overworked. The main cooling unit's valve works overtime to handle the heat surge.

BUSINESS VALUE

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BUSINESS VALUE

Area	Value Delivered
Proactive Fault Detection	Early alarms, reduced scrap, fewer shutdowns, better product quality
Process Automation	Automated monitoring, reduced operator burden, foundation for Industry 4.0
Operations and Maintenance Planning	Predictive maintenance, targeted interventions, longer equipment life
Emergency Planning	Faster escalation decisions, safer operation, reduced accident probability

LIMITATIONS

- Domain Knowledge Required Models detect anomalies, but interpretation and decisions depend on plant expertise.

- Detection ≠ Action. Actual responses depend on risk, safety, and operations strategy.

- Analytics should support, not replace engineering heuristics and judgment

APPENDICES

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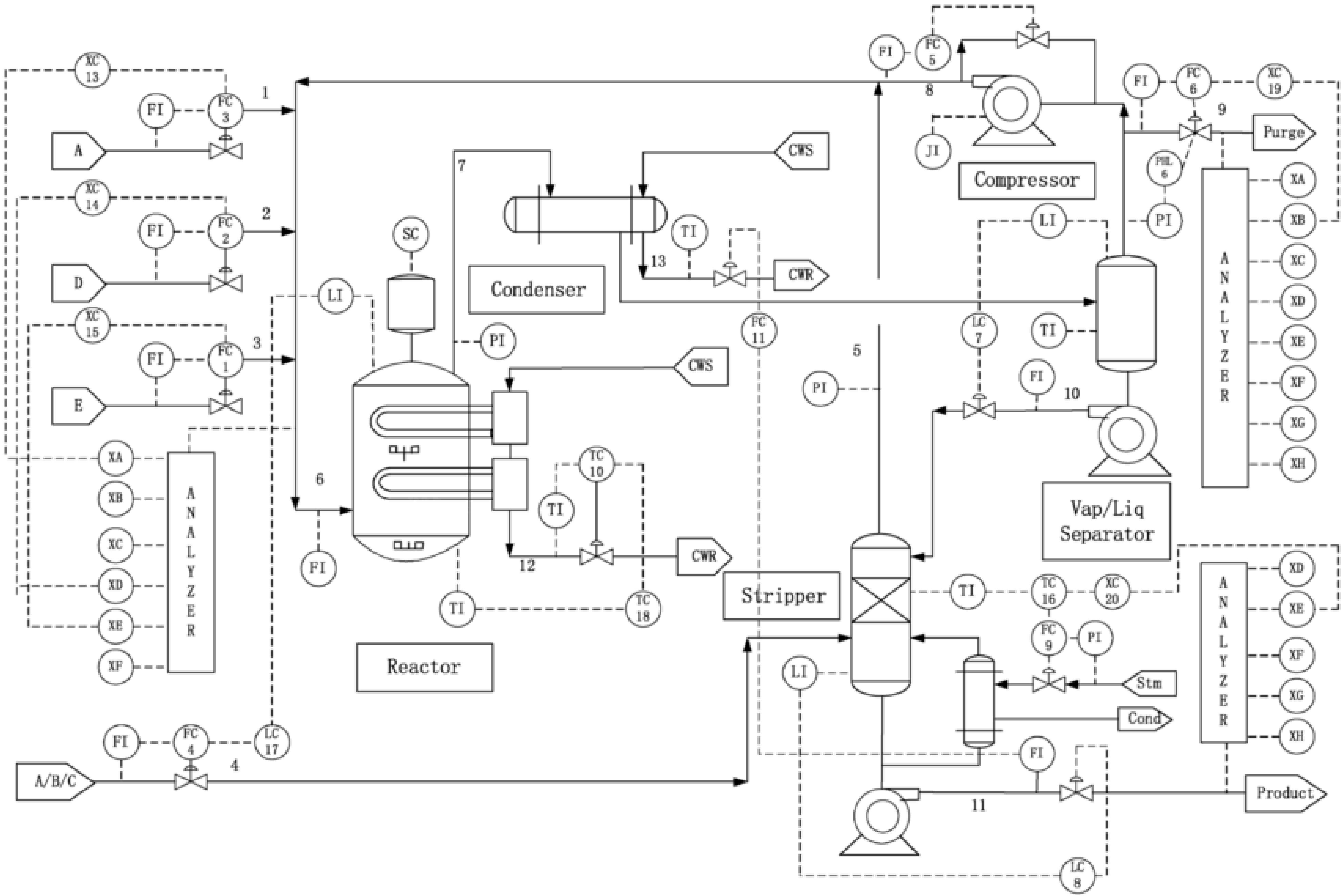
PROCESS FLOW DIAGRAM



TEP Fault Types
Status (1-20)

A. Process Faults

- Fault 1 – Step change in A/C feed ratio

(Feed stream 4 composition changes: ratio of Component A to Component C)

- Fault 2 – Step change in Feed B composition

(Composition of Stream 2 suddenly changes)

- Fault 3 – Step change in Feed D composition

(Composition of Stream 3 suddenly changes)

- Fault 4 – Step change in Feed E composition

(Composition of Stream 1 changes)

- Fault 5 – Feed A temperature variation

Step change or sustained variation in Feed A temperature.

- Fault 6 – Feed B temperature variation

Step change in Feed B temperature.

- Fault 7 – Feed C temperature variation

Step change in Feed C temperature.

- Fault 8 – Feed D temperature variation

Step change in Feed D temperature.

- Fault 9 – Condenser cooling water inlet temperature variation

Cooling water temperature changes → affects condenser efficiency.

B. Mechanical Faults

- Fault 10 – Reactor cooling water valve stuck

Cooling water flow to the reactor becomes fixed.

- Fault 11 – Condenser cooling water valve stuck

Cooling water flow to the condenser becomes fixed.

- Fault 12 – A feed valve stuck

Feed A flow cannot change (control failure).

- Fault 13 – D feed valve stuck

Feed D flow cannot change.

- Fault 14 – Separator pot liquid level valve stuck

Level control loop failure.

- Fault 15 – Stripper steam valve stuck

Steam supply to stripper fixed.

B. Random/Stochastic Faults

- Fault 16 – Random variation in reactor cooling water temperature
- Fault 17 – Random variation in condenser cooling water temperature
- Fault 18 – Random variation in feed A composition
- Fault 19 – Random variation in feed B composition
- Fault 20 – Random variation in feed A temperature

Measured Variables
XMEAS (1-41)

A. Feeds & Flow Rates
- XMEAS(1) – A feed (stream 1)
- XMEAS(2) – D feed (stream 2)
- XMEAS(3) – E feed (stream 3)
- XMEAS(4) – Total feed (stream 4)
- XMEAS(5) – Recycle flow (stream 8)
- XMEAS(6) – Reactor feed rate (stream 6)
- XMEAS(10) – Purge rate (stream 9)
- XMEAS(14) – Separator underflow (stream 10)
- XMEAS(17) – Stripper underflow (stream 11)
- XMEAS(19) – Stripper steam flow
- XMEAS(20) – Compressor work

B. Reactor
- XMEAS(7) – Reactor pressure
- XMEAS(8) – Reactor level
- XMEAS(9) – Reactor temperature
- XMEAS(21) – Reactor cooling-water outlet temperature

C. Separator & Condenser
- XMEAS(11) – Separator temperature
- XMEAS(12) – Separator level
- XMEAS(13) – Separator pressure
- XMEAS(22) – Condenser cooling-water outlet temperature

D. Stripper
- XMEAS(15) – Stripper level
- XMEAS(16) – Stripper pressure
- XMEAS(18) – Stripper temperature

E. Product Composition
Stream 6 (reactor outlet)
- XMEAS(23) – A, (24) – B, (25) – C
- XMEAS(26) – D, (27) – E, (28) – F

F. Product Composition
Stream 11 (bottoms / product)
- XMEAS(37) – D, (38) – E, (39) – F
- XMEAS(40) – G, (41) – H

Manipulated Variables
XMV (1-12)

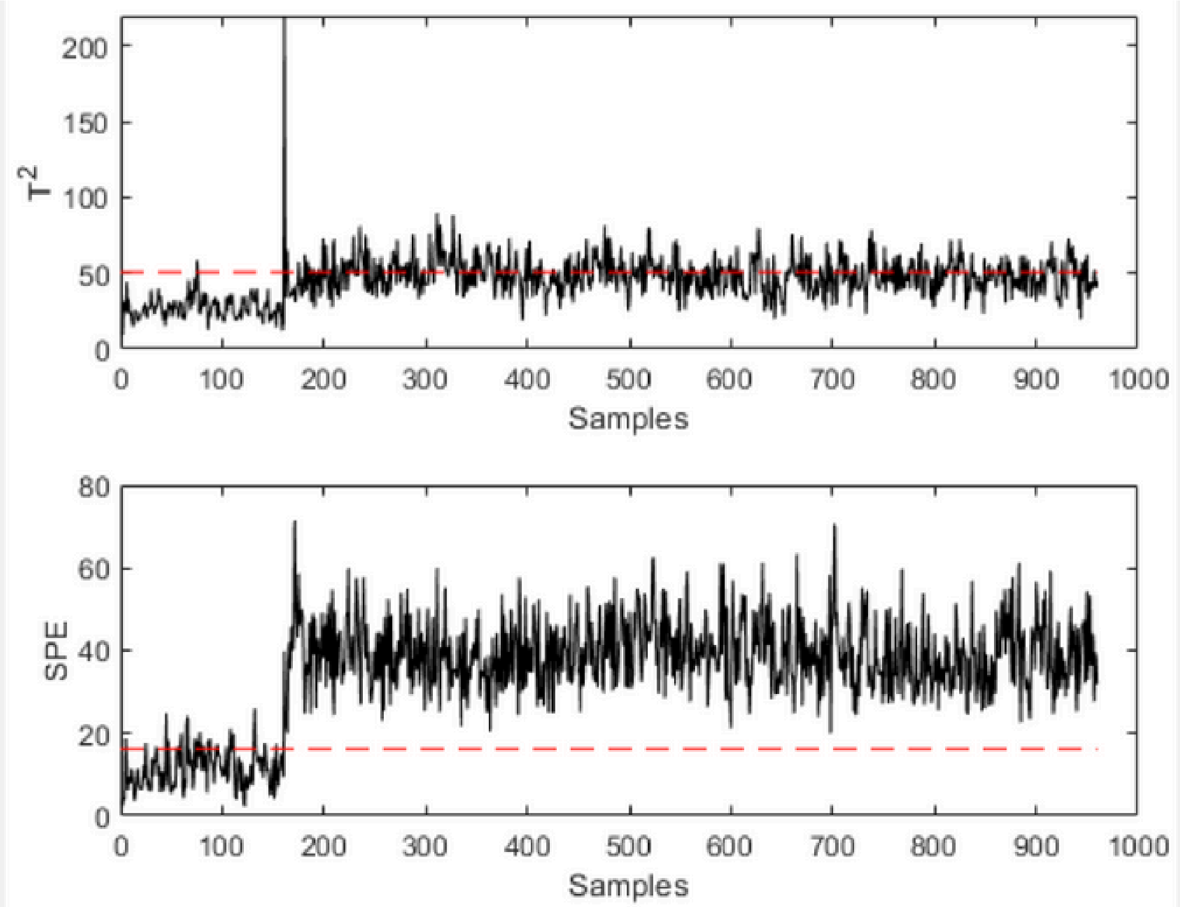
G. Feed & Flow Control
- XMV(1) – D feed flow (stream 2)
- XMV(2) – E feed flow (stream 3)
- XMV(3) – A feed flow (stream 1)
- XMV(4) – Total feed flow (stream 4)
- XMV(5) – Compressor recycle valve
- XMV(6) – Purge valve (stream 9)
- XMV(7) – Separator pot liquid flow (stream 10)
- XMV(8) – Stripper liquid product flow

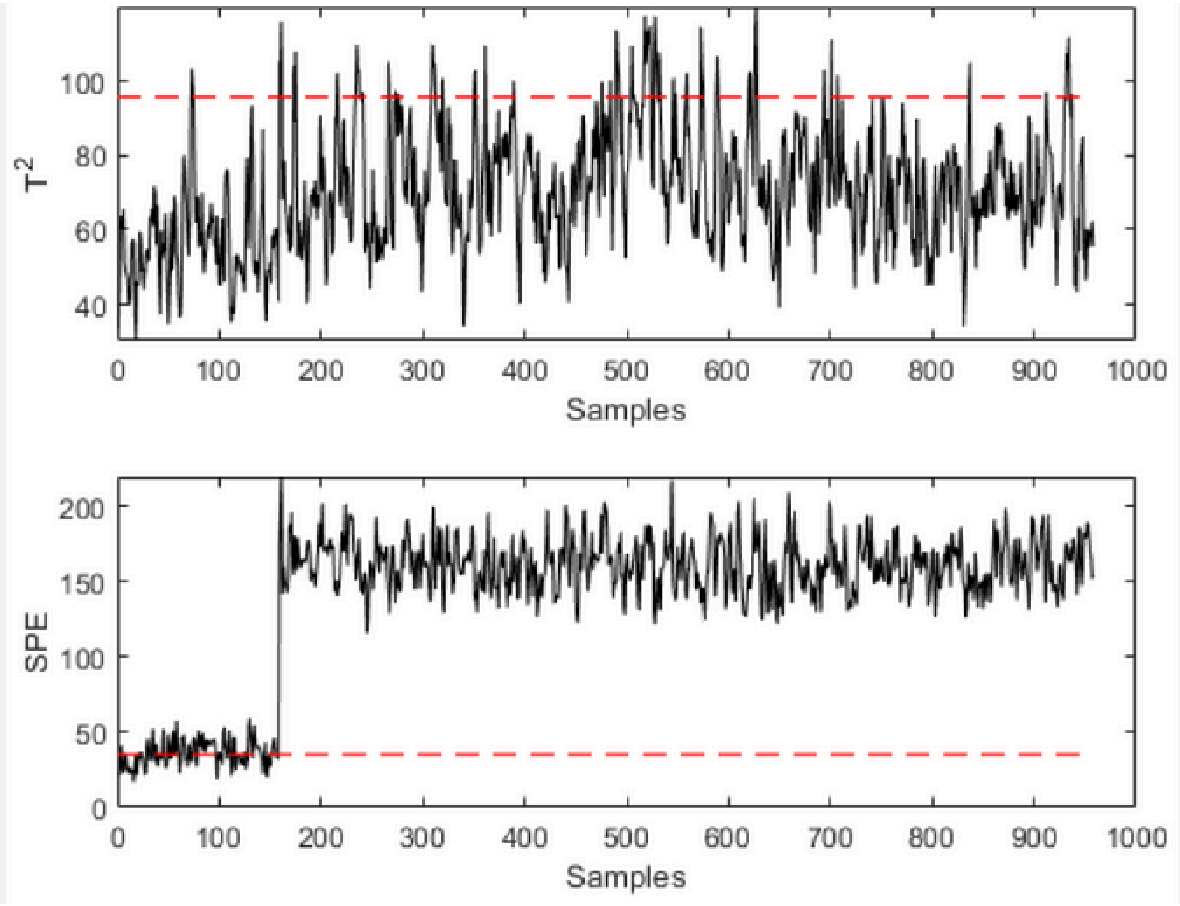
H. Cooling & Utility Control
- XMV(9) – Stripper steam valve
- XMV(10) – Reactor cooling-water flow
- XMV(11) – Condenser cooling-water flow
- XMV(12) – Agitator speed petertino.github.io

THEORETICAL FRAMEWORK

FAULT DETECTION

Takens-PCA (Dynamic PCA)





Fault Diagnosis Using Dynamic Principal Component Analysis and GA Feature Selection Modeling for Industri...

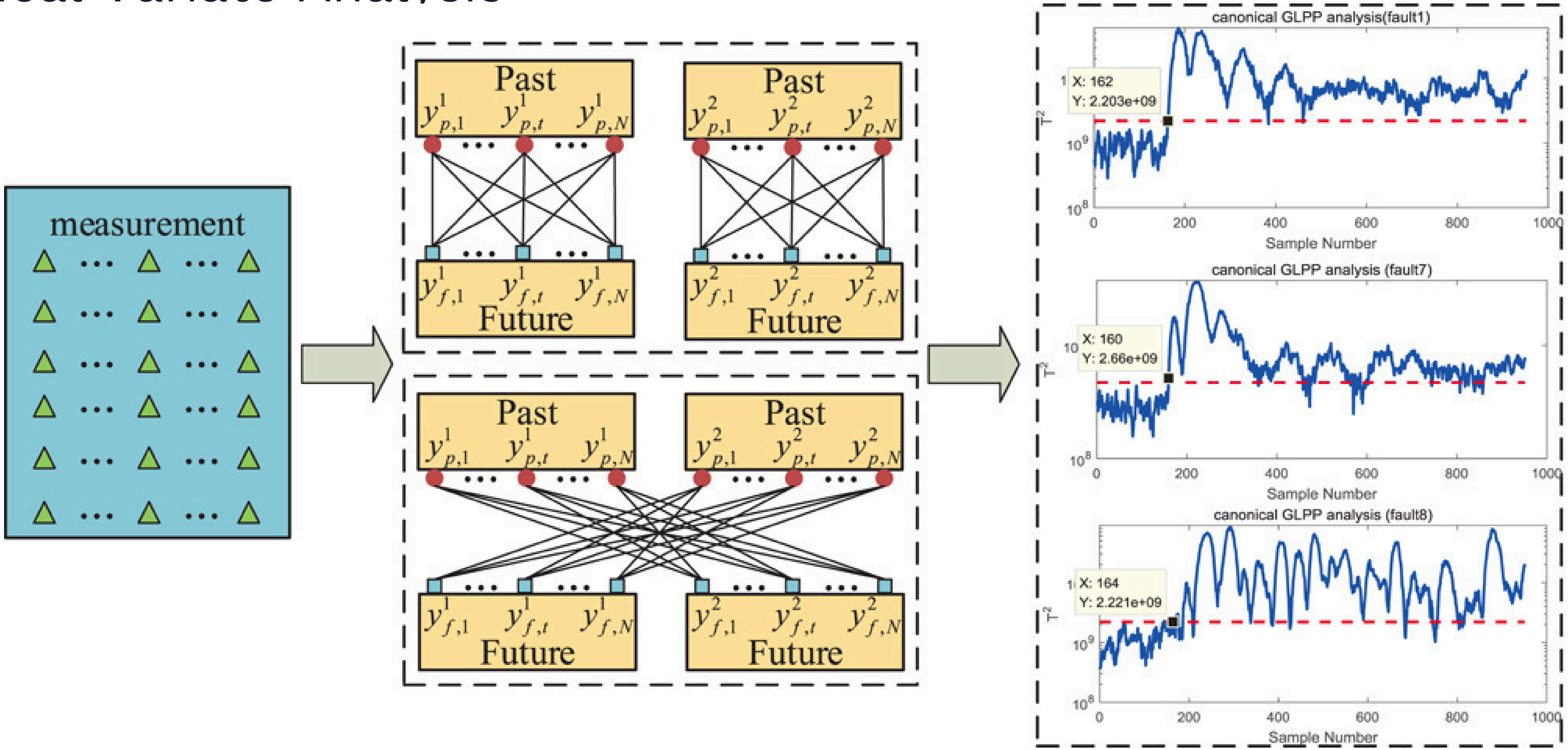
With the continuous expansion of industrial production scale, most of the chemical process variables are nonlinear, multi-modal and dynamic.

MDPI / Dec 2, 2022

THEORETICAL FRAMEWORK

FAULT DETECTION

Canonical Variate Analysis



THEORETICAL FRAMEWORK

FAULT DETECTION

(PDF) Canonical Variate Dissimilarity Analysis for Proces...

PDF | Early detection of incipient faults in industrial processes is increasingly...

ResearchGate

Canonical Variate Dissimilarity Analysis

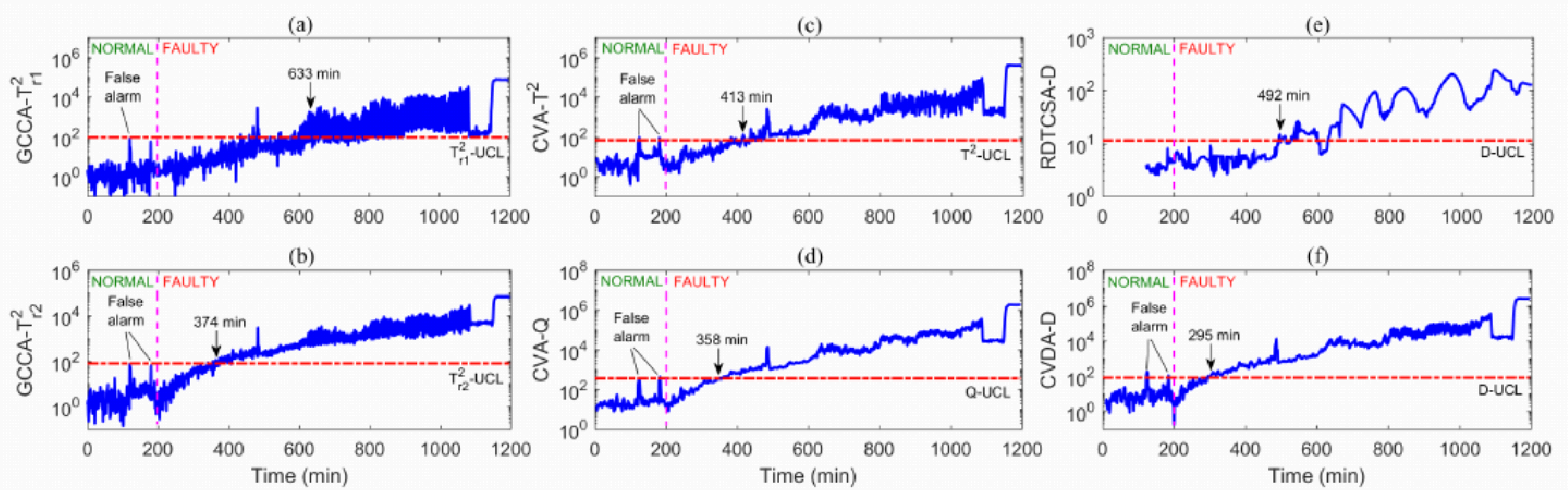
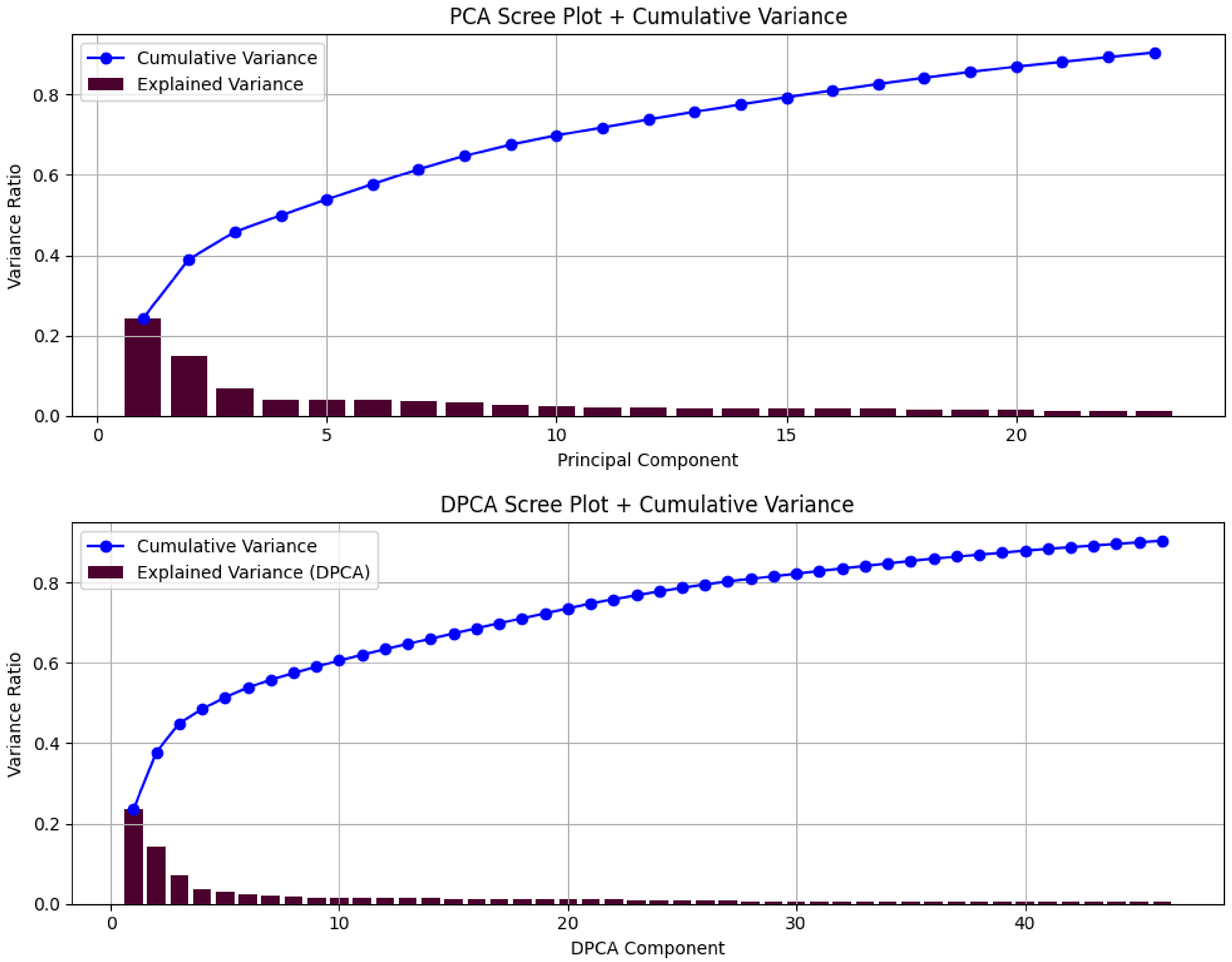


Fig. 6. Monitoring charts for Fault 3 using: (a,b) GCCA; (c,d) CVA; (e) RDTCSA; (f) CVDA. See Section IVc for implementation details. Legend: Dashdot - upper control limit (UCL); Dash - start of fault; Solid - detection index.

SCREE & CUMULATIVE VARIANCE PLOT



PCA sees the big changes, but DPCA sees the slow, hidden changes, which is why **DPCA is better for detecting early faults**.

THEORETICAL FRAMEWORK

FAULT DETECTION

Detection Methods

Method	Original Variables	Intermediate Variables (After Lags)	Final Components Kept	Explained Variance
PCA	52	N/A (Static)	23	90.46%
DPCA	52	156	46	90.36%
CVA	52	260 (p=5, f=5)	20	N/A
CVDA	52	N/A (filter/pre-processor)	N/A	N/A

FAULT BEHAVIOR LIBRARY

Fault No.	Fault Description	Top Contributing Variables	Implications
1	Feed A/C Ratio Change (Composition)	XMEAS(23), XMEAS(38) (Product Composition)	Product Purity is wrong. The final chemical mix is immediately different.
2	Feed B Composition Change	XMEAS(15), XMV(8) (Stripper Level/Flow)	The Stripper Level is unstable. The liquid separation unit goes haywire.
3	Feed D Composition Change	XMV(1), XMEAS(2) (D Feed Flow/Valve)	D Feed Valve is compensating hard. The controls are frantically adjusting D Feed flow to fix the mix.
4	Feed E Composition Change	XMV(10) (Reactor Cooling-Water Flow)	Reactor is too hot/cold. The main cooling valve has to slam open or shut due to the heat change.
5	Feed A Temperature Variation	XMV(11) (Condenser Cooling-Water Flow)	Condenser is overworked. The main cooling unit's valve works overtime to handle the heat surge.

FAULT BEHAVIOR LIBRARY

Fault No.	Fault Description	Top Contributing Variables	Implications
6	Feed B Temperature Variation	XMV(3), XMEAS(1) (A Feed Flow/Valve)	A Feed Valve is compensating. The system is trying to fix the heat issue by changing the A Feed flow.
7	Feed C Temperature Variation	XMEAS(27) (E Comp.), XMEAS(8) (Reactor Level)	Reactor Level is moving. The change in density/volume causes the Reactor liquid level to swing.
8	Feed D Temperature Variation	XMEAS(23) (A Comp.), XMEAS(8) (Reactor Level)	Reactor Level is moving and the product mix is changing.
9	Condenser Cooling Water Inlet Temp Variation	XMV(1), XMEAS(2) (D Feed Flow/Valve)	D Feed Valve is compensating. The system is adjusting D Feed to handle the poor cooling efficiency.
10	Reactor Cooling Valve Stuck (EME)	XMV(10) (Reactor Cooling-Water Flow)	The Stuck Valve screams. The variable that is fixed (XMV(10)) is the clearest sign of its own failure.

FAULT BEHAVIOR LIBRARY

Fault No.	Fault Description	Top Contributing Variables	Implications
11	Condenser Cooling Valve Stuck (EME)	XMV(10) (Reactor Cooling-Water Flow)	Reactor Cooling tries to compensate. The Reactor's cooling valve (XMV(10)) is forced to overwork because the downstream Condenser is broken.
12	A Feed Valve Stuck (EME)	XMEAS(11) (Separator Temperature)	Separator Temperature goes wild. Fixing the largest feed flow destabilizes the separator unit completely.
13	D Feed Valve Stuck (EME)	XMEAS(16) (Stripper Pressure), XMEAS(23) (A Comp.)	Stripper Pressure and Product Mix are wrong. Cannot control D Feed, messing up the separation unit.
14	Separator Liquid Level Valve Stuck (EME)	XMEAS(21) (Reactor Cooling-Water Outlet Temp)	Reactor Cooling load spikes. The blockage in the separator disrupts the recycle flow, impacting the Reactor's cooling.
15	Stripper Steam Valve Stuck (EME)	XMV(1), XMEAS(2) (D Feed Flow/Valve)	D Feed Valve is compensating. The control system adjusts D Feed to counteract the fixed steam/poor separation.

FAULT BEHAVIOR LIBRARY

Fault No.	Fault Description	Top Contributing Variables	Implications
16	Random Variation in Reactor Cooling Temp	XMV(1), XMEAS(2) (D Feed Flow/Valve)	D Feed Valve is compensating. The system adjusts D Feed to manage the sudden heat fluctuations in the reactor.
17	Random Variation in Condenser Cooling Temp	XMEAS(21) (Reactor Cooling-Water Outlet Temp)	The Reactor feels the heat. The cooling change at the Condenser comes back via the recycle stream to affect the Reactor.
18	Random Variation in Feed A Composition	XMEAS(11) (Separator Temp), XMEAS(22) (Condenser C/W Outlet Temp)	Separator/Condenser are disrupted. The changing mix in Feed A causes temperature swings in the downstream separation units.
19	Random Variation in Feed B Composition	XMV(1), XMEAS(2) (D Feed Flow/Valve)	D Feed Valve is compensating. The control system adjusts D Feed to balance the effects of the changing Feed B mix.
20	Random Variation in Feed A Temperature	XMV(5) (Compressor Recycle Valve)	Recycle Gas Valve is swinging wildly. The temperature change in Feed A changes the gas flow, making the pressure control valve (XMV(5)) react instantly.

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