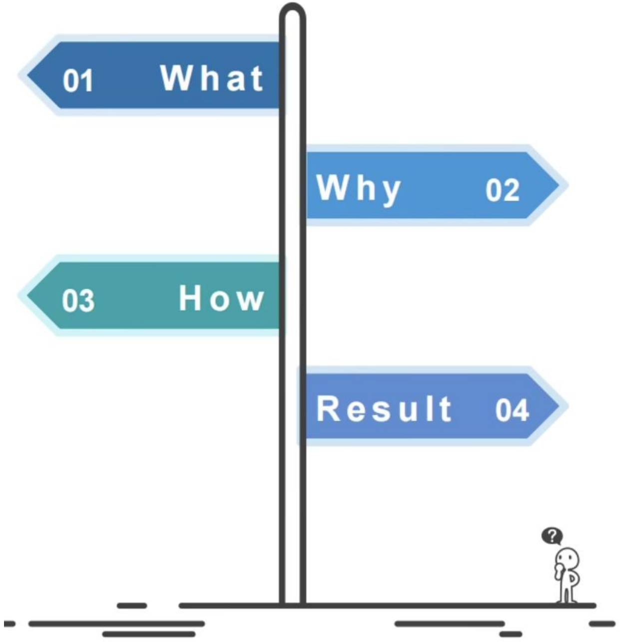
Leakage diagnosis of hydrogen synthesis process with the MDD-RF methods

H2021702 （QIN LIZHEN）

New energy lab

CONTENTS



Background

a. Importance of safety in chemical processes:

- ➢ **Human Health Preservation****: Safety measures protect workers from exposure to hazardous materials, reducing the risk of accidents and long-term health issues.
- ➢ **Environmental Conservation****: Safety protocols minimize pollution and environmental damage caused by chemical spills or emissions, preserving ecosystems.
- ➢ **Asset Safeguarding****: Safety practices prevent equipment failures and production interruptions, safeguarding costly assets and maintaining operational efficiency.

Background

b. Limitations of traditional leakage diagnosis methods

- Traditional methods may **not capture the complexities of dynamic chemical processes** adequately.
- They often rely on static assumptions and simplified models.
- Traditional methods may overlook critical factors such as fluctuating concentrations of reactive species.
- Complex interactions and non-linear behaviors may be challenging to account for.

1. **Gas Sensor Detection Method**:
- - **Disadvantages**: Relies on specific sensors, prone to false alarms or misses, requires frequent calibration.

2. **Infrared Imaging Detection Method**:
- - **Disadvantages**: High cost, susceptible to environmental conditions and background interference.

c. significance of dynamic simulation and random forest for leakage diagnosis

- Innovative Algorithm Proposal: The research aims to introduce an innovative MDD-RF (Modelica Dynamic Data - Random Forest) integrated algorithm for diagnosing leaks in hydrogen synthesis processes.
- Optimizing Process Control: Through feature importance analysis, the paper identifies key process parameters affecting leak prediction, providing guidance for further optimization of algorithm models and process control.
- Improved Diagnostic Accuracy and : In addition to diagnosing leak faults, the algorithm demonstrates high accuracy and robustness in diagnosing other common hydrogen synthesis fault modes.

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Methodology- The steady-state simulation system

Ammonia H2 Process Example 1,000 Nm3/hr Pilot

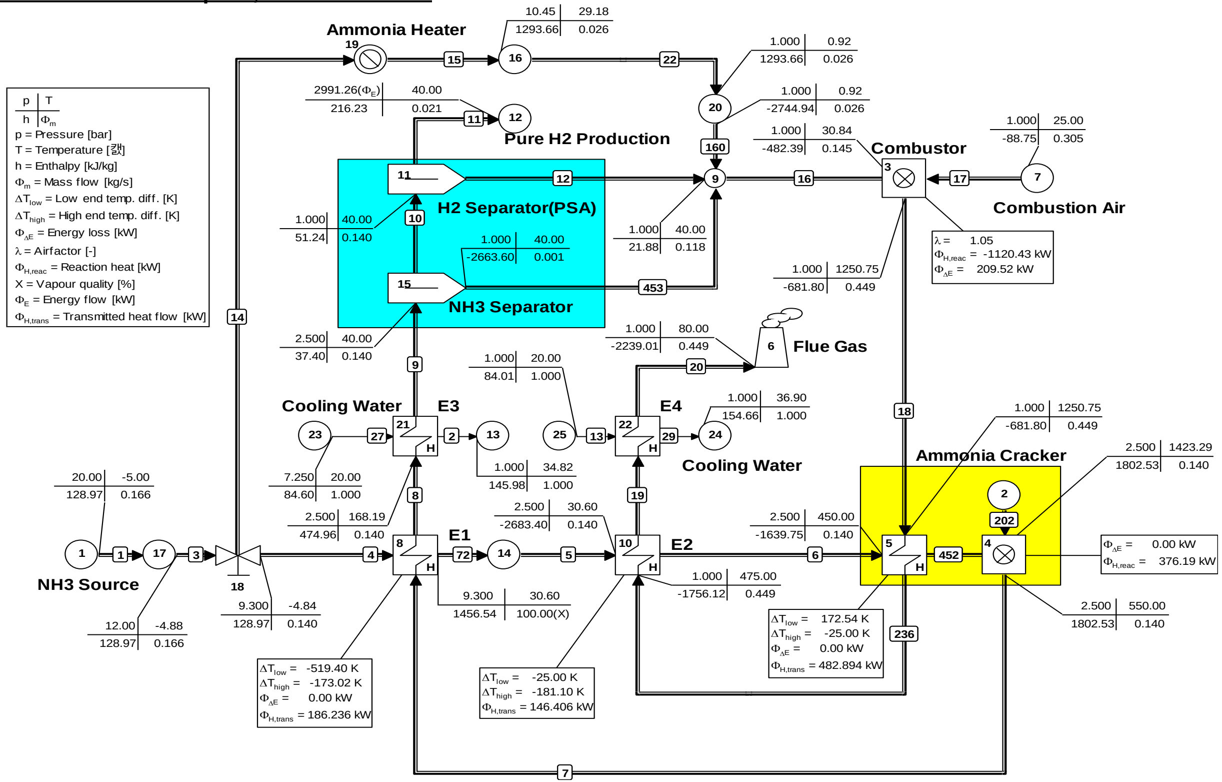


Figure 5. The steady-state simulation system of hydrogen synthesis was cycle-tempo.

Methodology-Simulation and comparison results of hydrogen synthesis process

Stream Empty Cell	Temperature (℃)			Pressure (MPa)			Mole flows (kg/s)			Composition				
	Simulation value	Reality value	Relative error %	Simulation value	Reality value	Relative error %	Simulation value	Reality value	Relative error	NH_3	N_2	O_2	H_2O	H_2
1	-5	-5	0	20	20	0	0.166	0.166	0	1	0	0	0	0
5	30.6	30		2.5	9.3		0.14	0.14	0	1	0	0	0	0
6	450	450		2.5	8.6		0.14	0.14	0	1	0	0	0	0
7	550	550		2.5	7.6		0.14	0.14	0	0.0026	0.2494	0	0	0.7481
8	168	166		2.5	7.45		0.14	0.14	0	0.0026	0.2494	0	0	0.7481
9	40	40		2.5	7.45		0.14	0.14	0	0.0026	0.2494	0	0	0.7481
10	40	40		1	6.1		0.14	0.14	0	0	0.25	0	0	0.75
11	40	40		1	5.8		0.021	0.02	0.001	0	0.0001	0	0	0.9999
12	40	40		1	0.5		0.118	0.12	0.02	0	0.69	0	0	0.31
16	30.84	40		1	1		0.145	0.14	0.005	0.1815	0.5644	0	0	0.254
17	25	25		1	1		0.305	0.3	0.005	0	0.7729	0.2075	0.0101	0
18	1250	1250		1	1		0.449	0.45	0.001	0.7486	0.0059	0.2397	0.0055	0

Methodology- Controller position for hydrogen synthesis process.

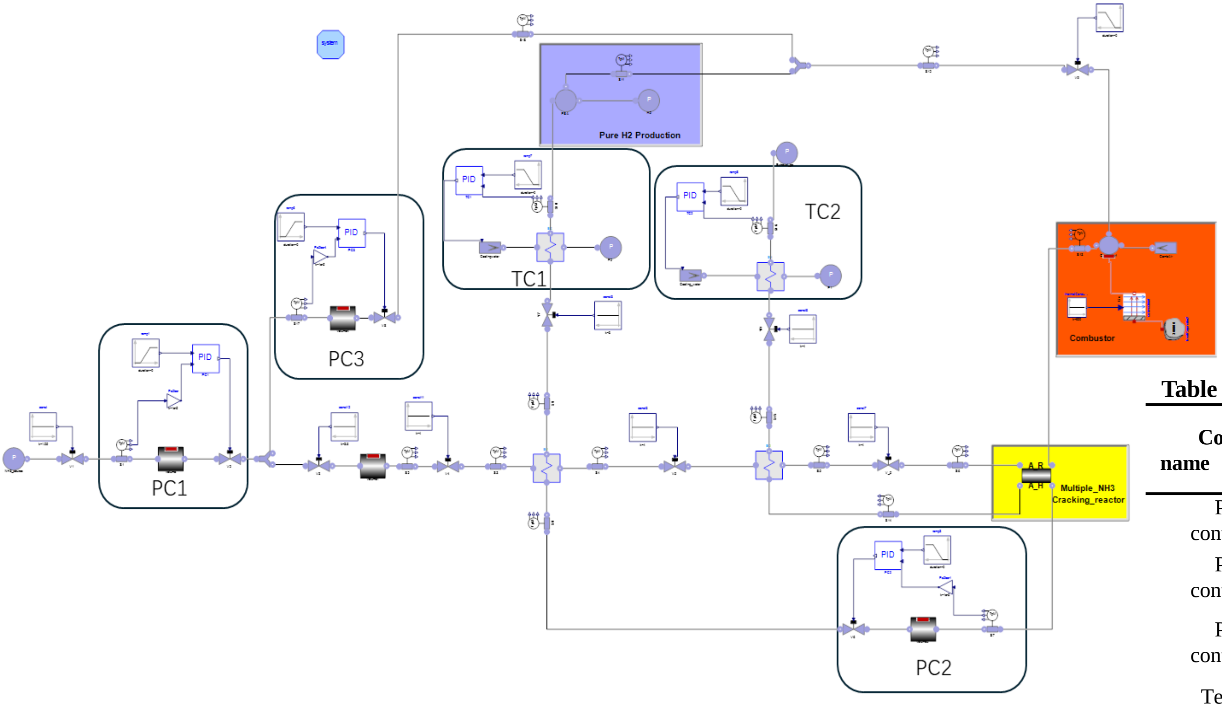


Fig. 6. Controller installation position for hydrogen synthesis process.

Table 3 Controller parameters.

Controller name	Tag number	Controlled variable	Manipulated variable	Target value
Pressure controller	PC1	Mainstream flow	V2 opening	12(bar)
Pressure controller	PC2	Ammonia cracker pressure	V6 opening	7.6(bar)
Pressure controller	PC3	Split flow	V8 opening	10(bar)
Temperature controller	TC1	PSA input temperature	Cooling water flow	313 (K)
Temperature controller	TC2	exhaust outlet temperature	Cooling water flow	353(K)

Methodology- Revised Hole Gas Leakage Model

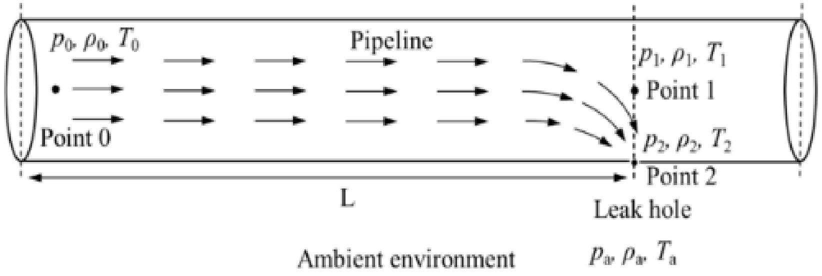
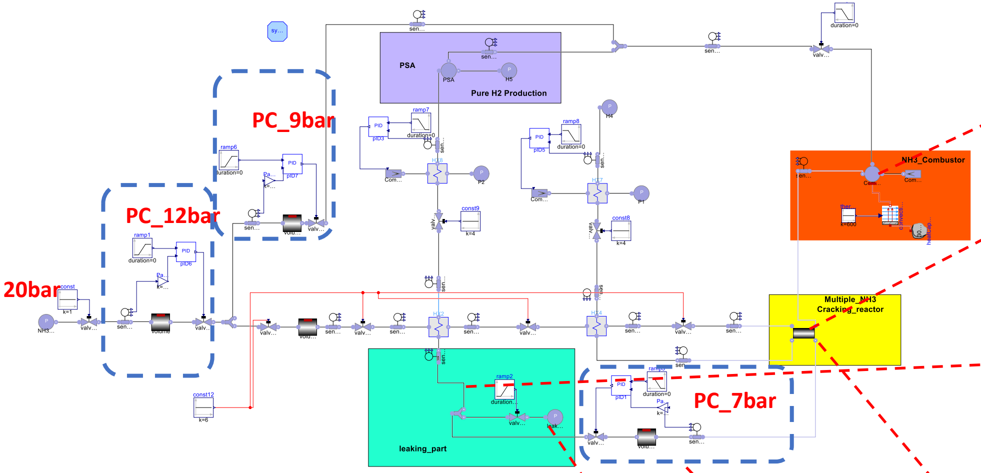


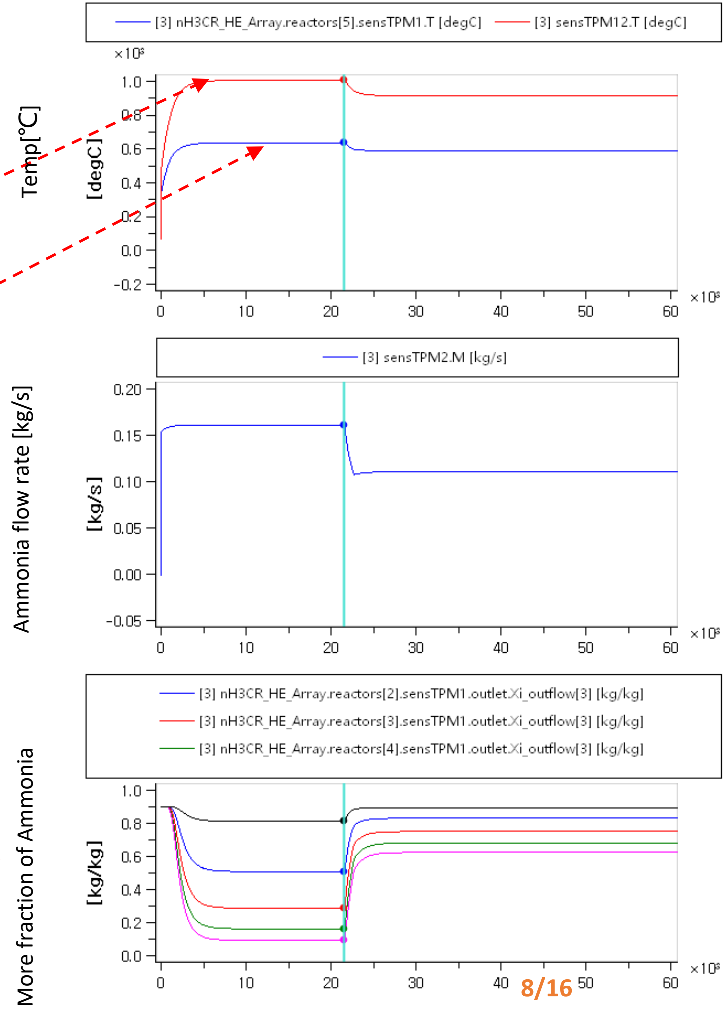
Figure 1. Schematic diagram of the gas leakage process in the hole model.

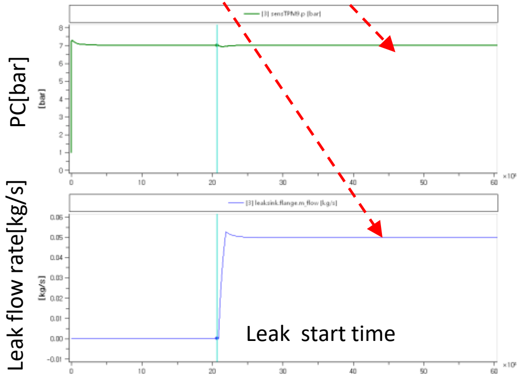
$$
\begin{cases}
CPR = \dfrac{p_a}{p_{cr}} = \left(\dfrac{2}{k+1}\right)^{\frac{k}{k-1}} \\
Q = \xi A_{or} p_1 \sqrt{\dfrac{kM}{RT_1}\left(\dfrac{2}{k+1}\right)^{\frac{k+1}{k-1}}} \quad p_1 \geq p_{cr} \text{ The gas is in sonic flow state} \\
Q = \xi A_{or} p_1 \sqrt{\dfrac{2k}{k-1}\dfrac{M}{RT_1}\left[\left(\dfrac{p_a}{p_1}\right)^{\frac{2}{k}} - \left(\dfrac{p_a}{p_1}\right)^{\frac{k+1}{k}}\right]} \quad p_1 < p_{cr} \text{ The gas is in subsonic flow state}
\end{cases}
$$

Ref: An Improved Gas Leakage Model and Research on the Leakage Field Strength Characteristics of R290 in Limited Space

Methodology- Abnormal simulation (leakage situation)







Methodology-leakage simulation

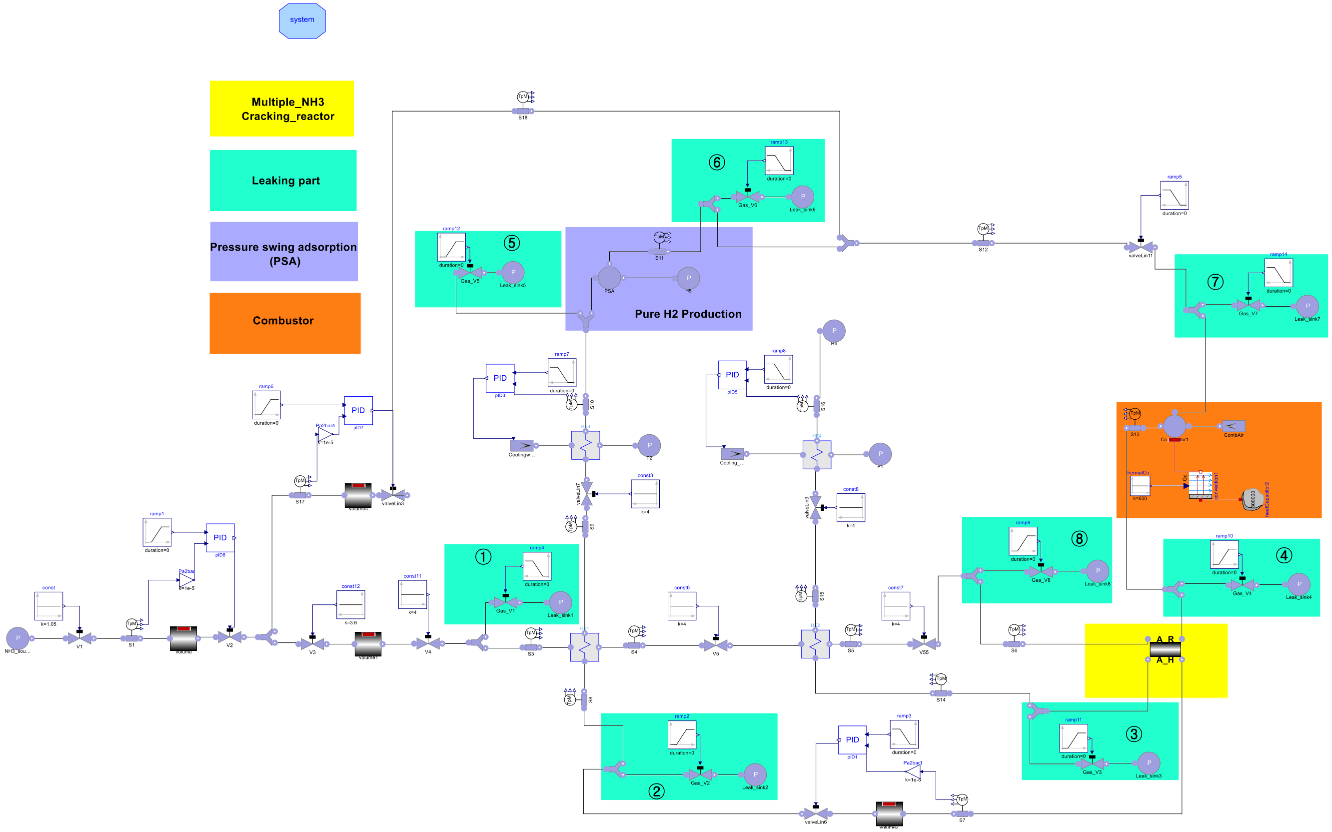
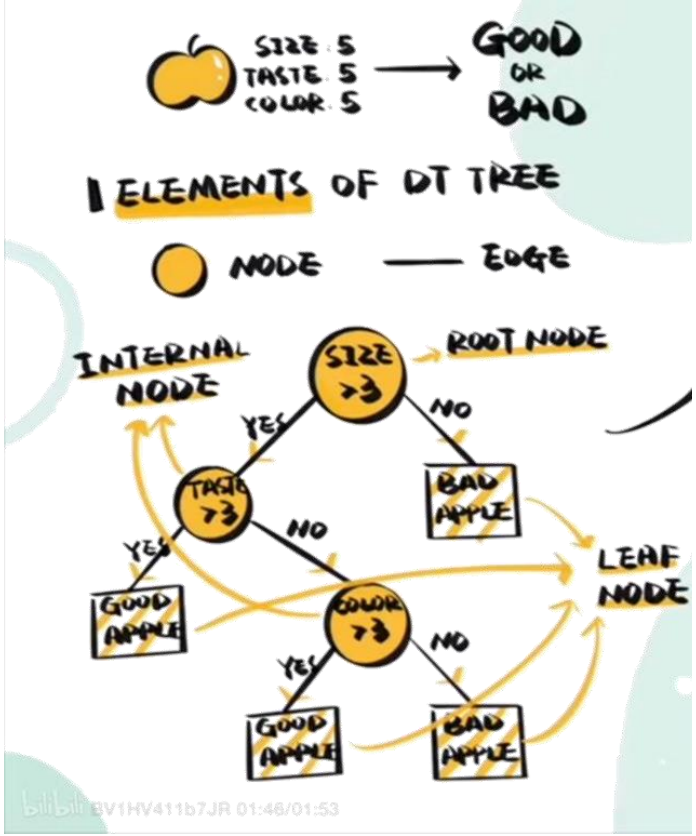
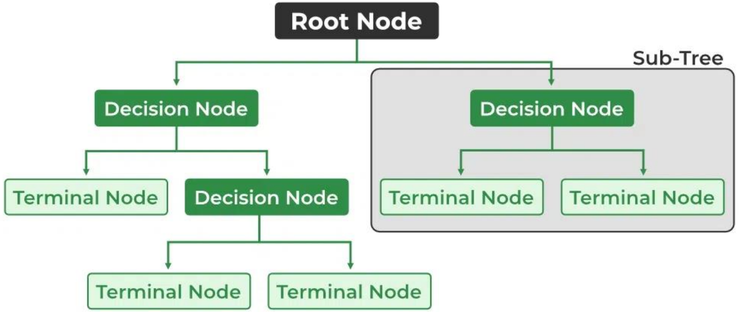


Figure 7 Schematic diagram of 8 possible leak points during the hydrogen synthesis process.

Methodology- Decision tree





- Table 1 Input variable description.

Variable	Symbol description	Variable	Symbol description	Variable	Symbol description
1	Combustor T [℃]	6	Branch flow[kg/s]	11	[H_2]_Mass fraction of [kg/kg]
2	Cracker T [℃]	7	Cracker pressure[bar]	12	PSA_In Cooling water flow[kg/s]
3	Combustor inlet flow[kg/s]	8	Combustor pressure[bar]	13	Ex_Gas Cooling water flow[kg/s]
4	Main inlet flow[kg/s]	9	[NH_3]_Mass fraction [kg/kg]	14	PSA_In Cooling water T[℃]
5	Cracker inlet flow[kg/s]	10	[N_2]_Mass fraction of [kg/kg]	15	PSA_In Cooling water T[℃]

Methodology- Construction of Decision Tree

Entropy

Entropy is a measure of the purity or disorder of a data set. In the decision tree algorithm, we want to divide the data set into subsets that are as "pure" as possible, that is, the instances in each subset belong to the same category.

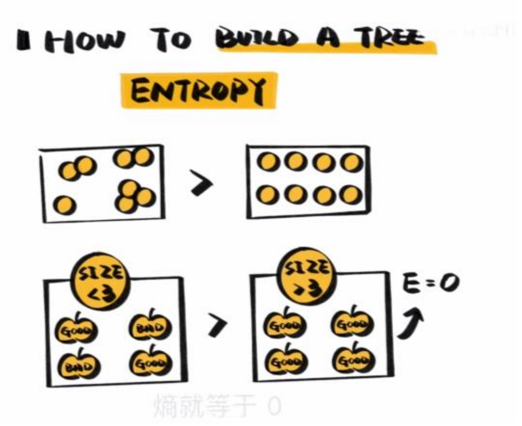
Entropy(S) = -Σ(p_i * log2(p_i))

in:

S is the data set

p_i is the proportion of S belonging to the i-th category

The higher the entropy value, the higher the degree of mixing and disorder of the data set.



Information Gain

Information gain describes the degree of entropy reduction after classifying a certain feature. The decision tree algorithm will select the feature with the largest information gain to split the data set.

Gain(S, A) = Entropy(S) - Σ(v=1 to V) (|S_v| / |S|) * Entropy(S_v)

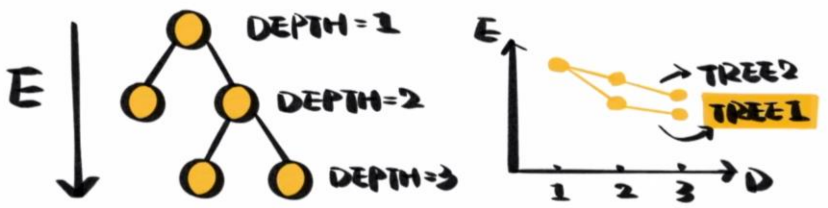
S is the data set

A is the feature to calculate the information gain

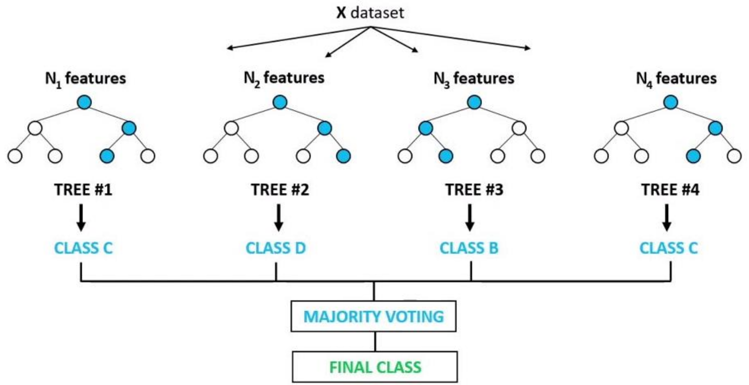
V is the number of different values of feature A

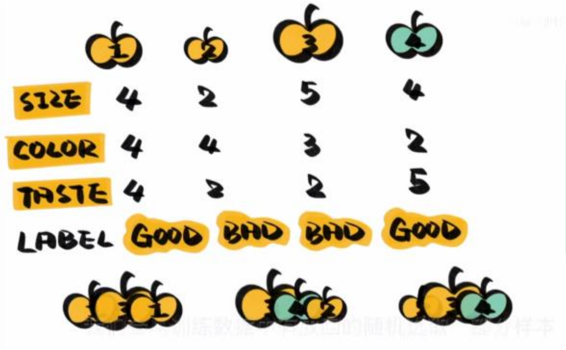
S_v is the subset of data set S when feature A takes the value v

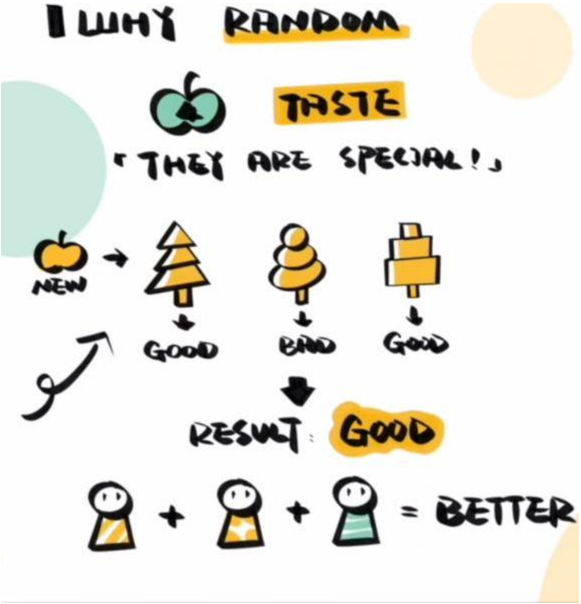
The greater the information gain, the lower the degree of disorder of the subset after using this feature for classification.



Methodology- Random forest







advantage

Methodology Process flow chart

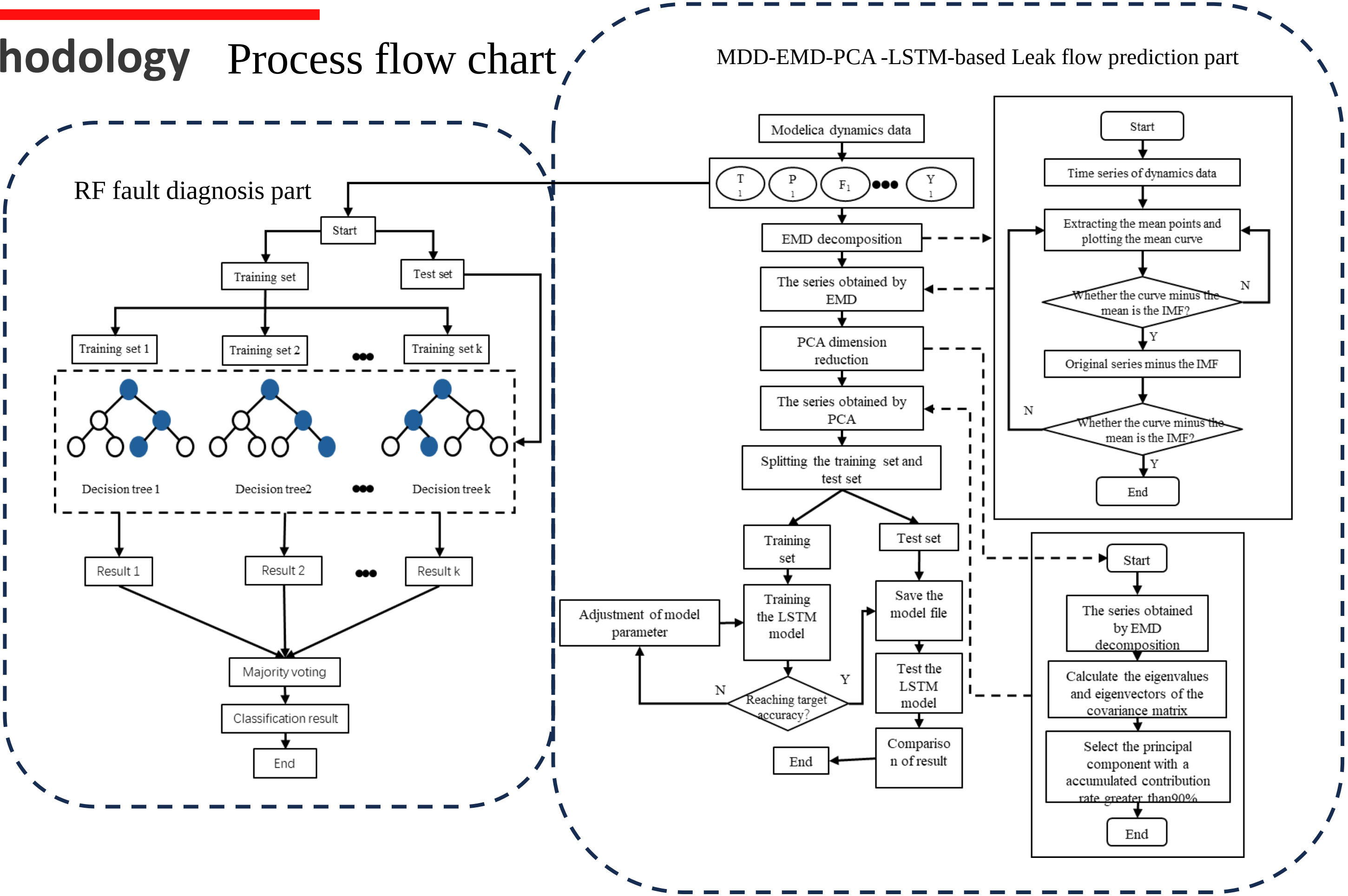
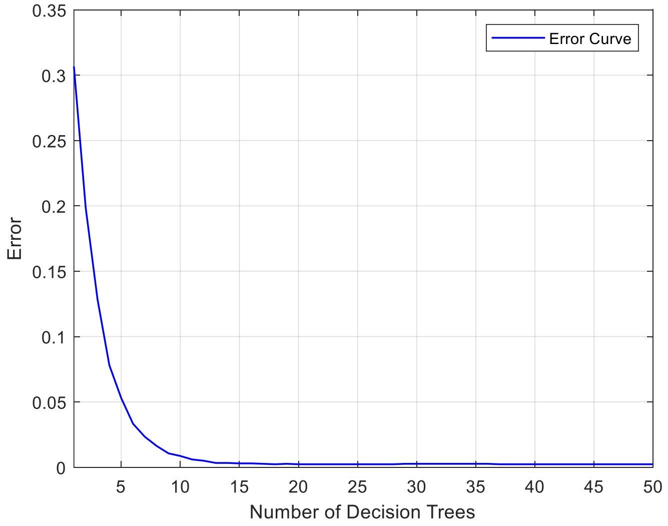
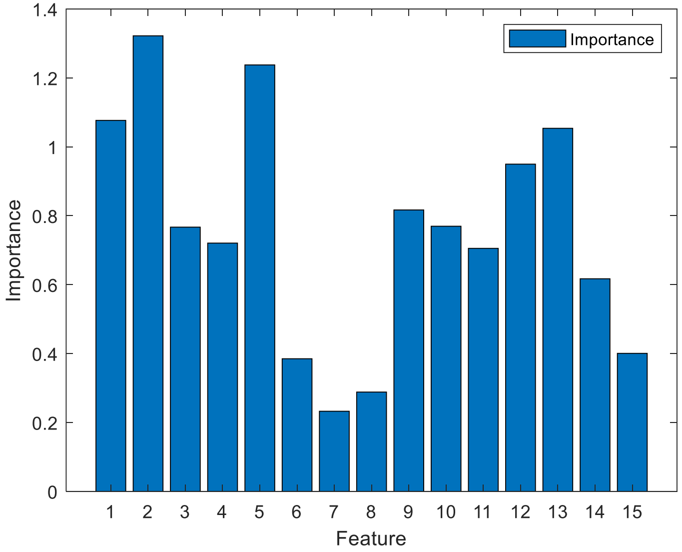


Figure. MDD-EMD-PCA -LSTM-based Leak flow prediction and MDD_RF-based fault diagnosis process flow chart.

Results Discriminant curve and feature Importance Plot





The discriminant curve is relatively smooth, indicating that the classifier has good discrimination ability for different categories of leakage faults.

By comparing the importance bar of different features, we can roughly judge which features are more critical and important to the classification prediction of the model

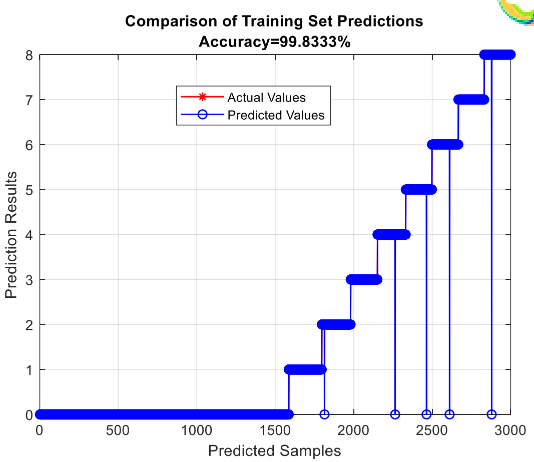
Results and conclusion

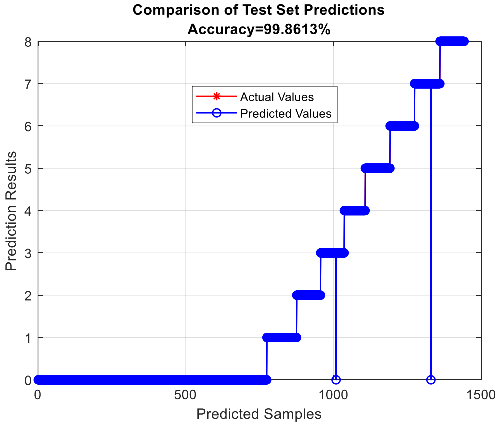
- Using an optimized random forest algorithm, this research achieved extremely high accuracy in leak detection and location prediction during the hydrogen synthesis process. The accuracy of leak location prediction is as high as 99.86%.

- Through feature importance analysis, it is determined that the two characteristics of cracking outlet temperature and main flow rate have the most critical impact on leakage location prediction, which provides guidance for further optimization of algorithms and systems.

- Our proposed MDD-RF models can not only successfully achieve leakage faults diagnosis but can also be extended to faults diagnosis in other fields, such as pipeline system fault and bearing fault diagnosis.

- Diversification and product integration: In addition to leak detection, there are opportunities to extend algorithms to diagnose various failure scenarios. By integrating algorithms with embedded devices, it becomes feasible to develop specialized detection products suitable for industrial use.





Leakage occurrence prediction results

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THE END

THANKS