Identify, Analyze, Optimize: Overcoming Energy Challenges in Chemical Engineering with Artificial Intelligence

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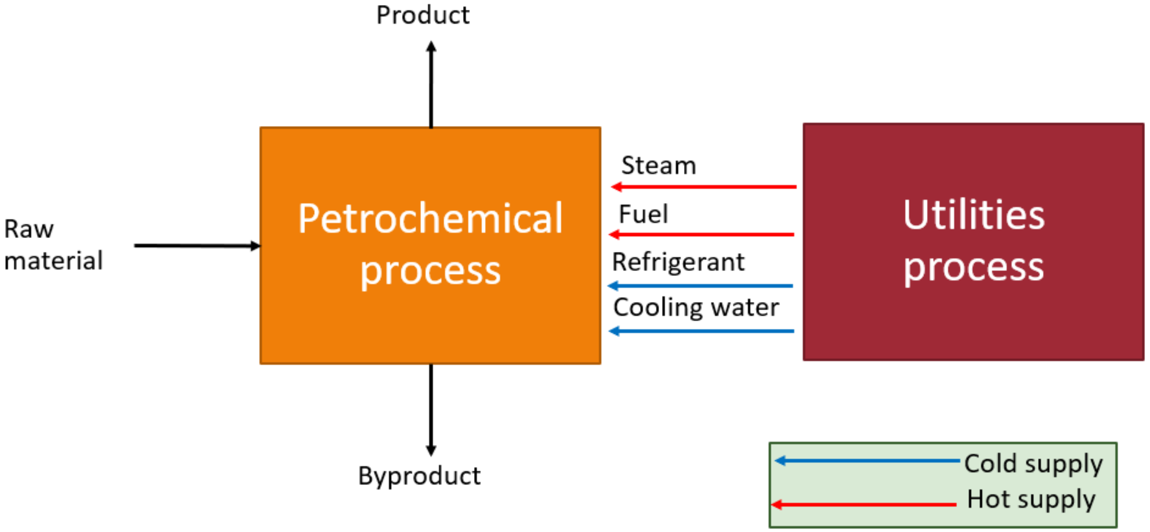
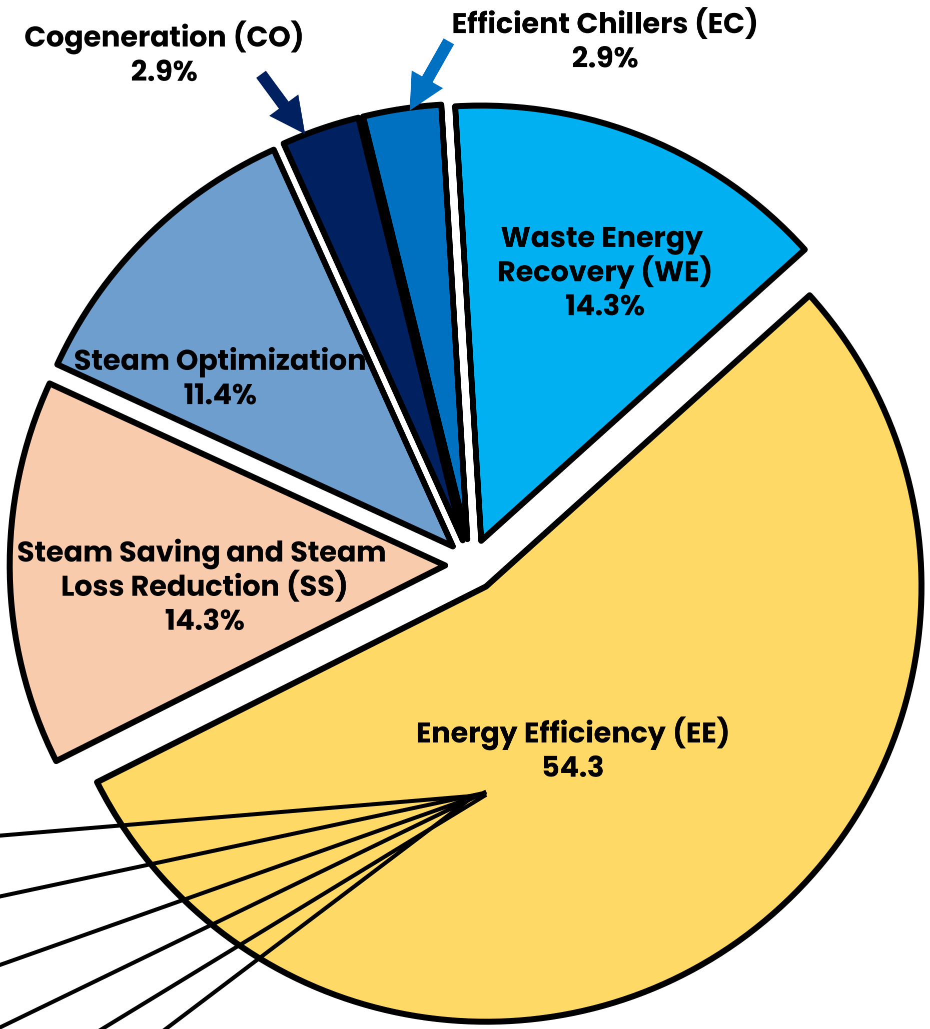
Introduction

Table 1 The framework for climate and energy – agreed targets

Years	Greenhouse Gas Emission	Energy Performance	Renewable Energy	Inter-Connection
2020	≤ -20%	≥ 20%	≥ 20%	10%
2030	≤ -40%	≥ 32.5%	≥ 32%	15%

Source : The European economic and social committee





Ensure access to affordable, reliable, sustainable and modern energy

Promote inclusive and sustainable economic growth by tracking production capacity

Build resilient infrastructure, promote sustainable industrialization and foster innovation

Make cities safe, resilient, and sustainable (Community related)

Ensure sustainable consumption and production patterns

Taking urgent action to tackle climate change and its impact

energy conservation measures in petrochemical industry, Thailand

Tantisattayakul et al. (2016), J. Clean. Prod.

Chemical engineering data challenges

Predictive Modeling

Process Data → Neural Network-Based Analysis → Energy Efficiency

Data Type

- **Continuous**
  - Operating Condition
- **Integer**
  - Process Variable
- **Categorical**
  - Type of catalyst
- **Binary/Boolean**
  - Sensor Status

Dimensionality

- **Time series data**
  - Online measurement of physical properties
- **Spatial data**
  - Spatial temperature distribution

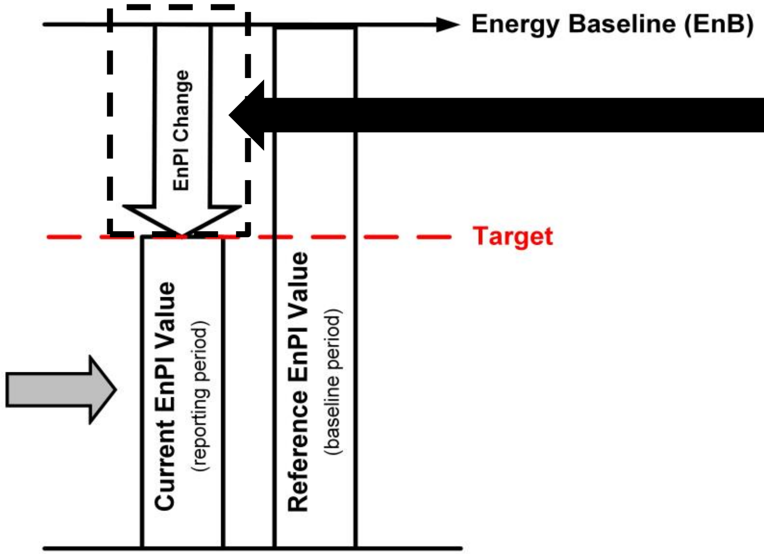
Reliability

- **Missing data**
  - Unknown states
  - Multi-rate information
  - Limited data
- **Corrupted data**
  - Drifting/Systematic errors
  - Sensor failure
- **Noisy data**
  - Poor measurement accuracy

Energy efficiency analysis

Energy Performance Indicators (EnPI)

- **Energy Consumption**
  e.g.: GJ, kWh
- **Energy Use**
  e.g.: Primary energy, electricity usage
- **Energy Efficiency**
  - Specific Energy Consumption (SEC)
  e.g.: GJ/ton, kWh/unit
  - Energy Intensity (EI)
  e.g.: GJ/$ GJ/Baht
  - Energy Conversion Efficiency
  e.g.: %



Chemical Process

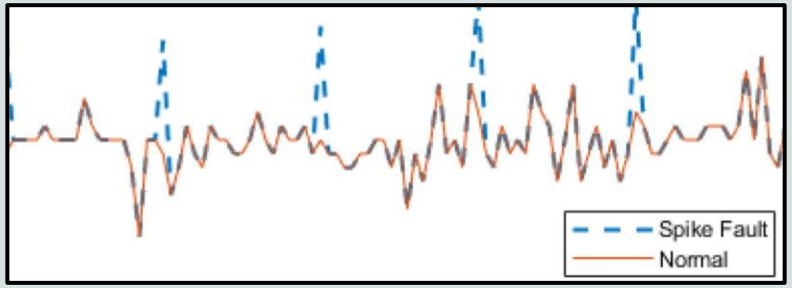
Reduce Energy Consumption

Increase Production Capacity

Specific Energy Consumption

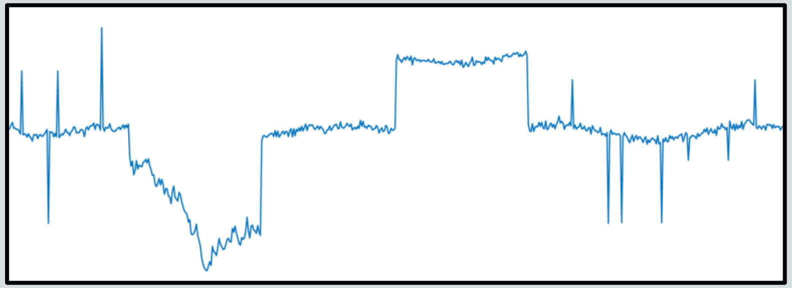
$$SEC = \frac{Energy\ used}{Production\ Capacity}$$

Uncertainty in chemical industry



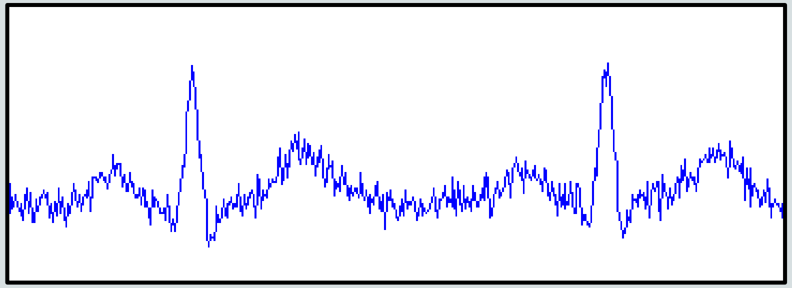
Measurement Fault

Jan et. al. (2020), Energy



Outlier

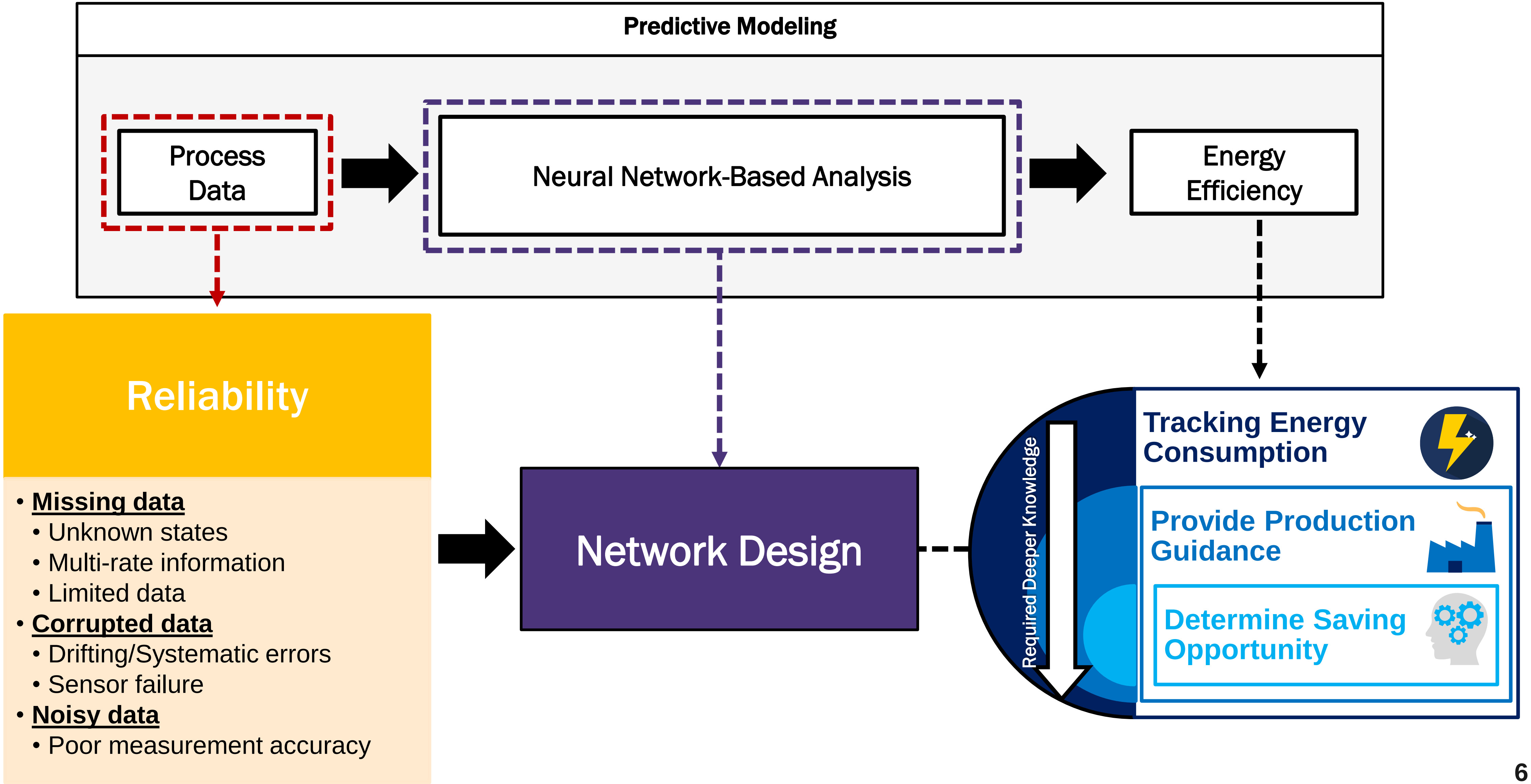
Xu et. Al. (2019), Neurocomputing



Operating Noise

Saeed et. al. (2021), Sensors

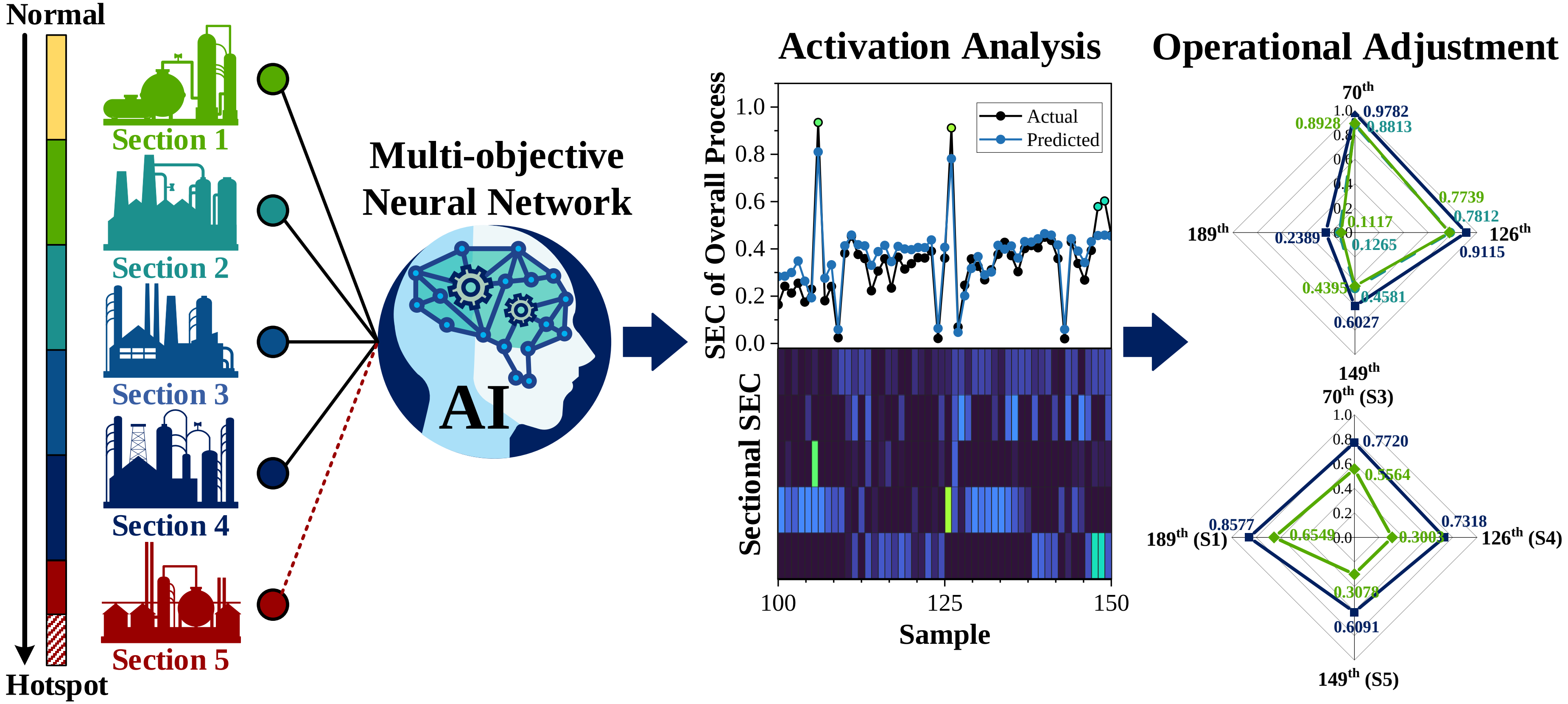
Neural network-based analysis



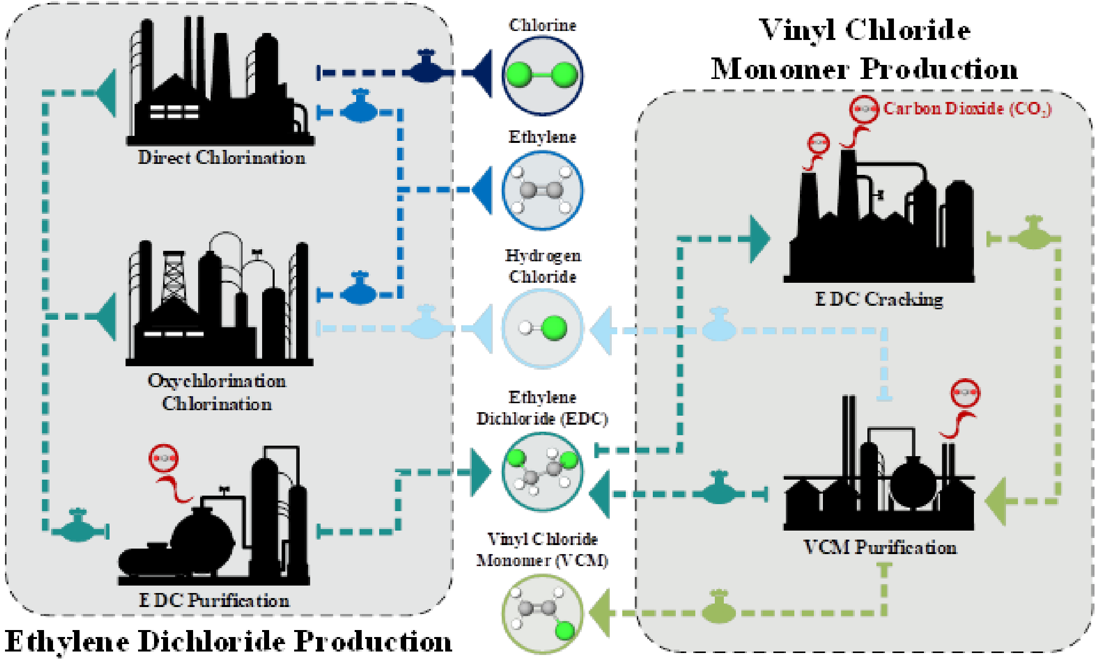
Energy hotspot identification

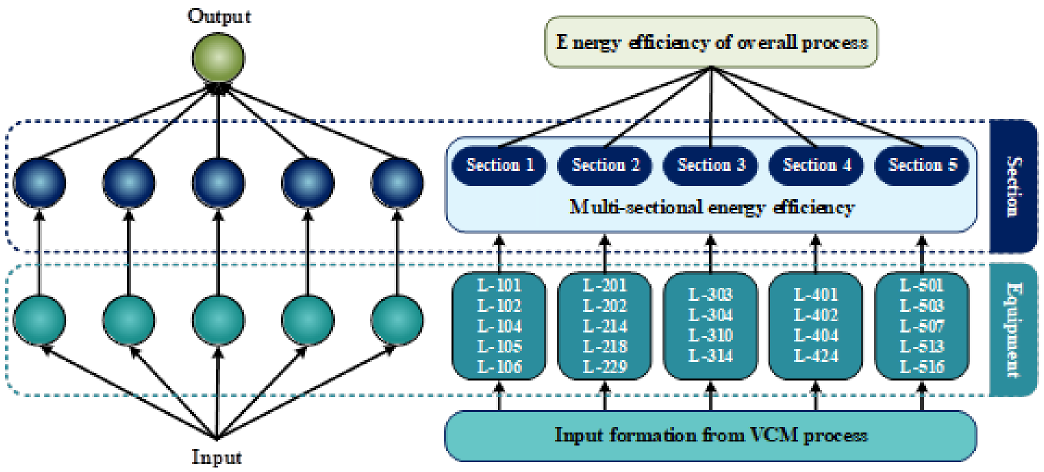
Energy hotspot identification framework

Process Information → **Multi-Objective Neural Network** → Objective 1 : Overall SEC / Objective 2 : Sectional SEC → **Operational Adjustment** → Improving Energy Efficiency, Resolve Energy Bottleneck



Energy efficiency model of VCM process





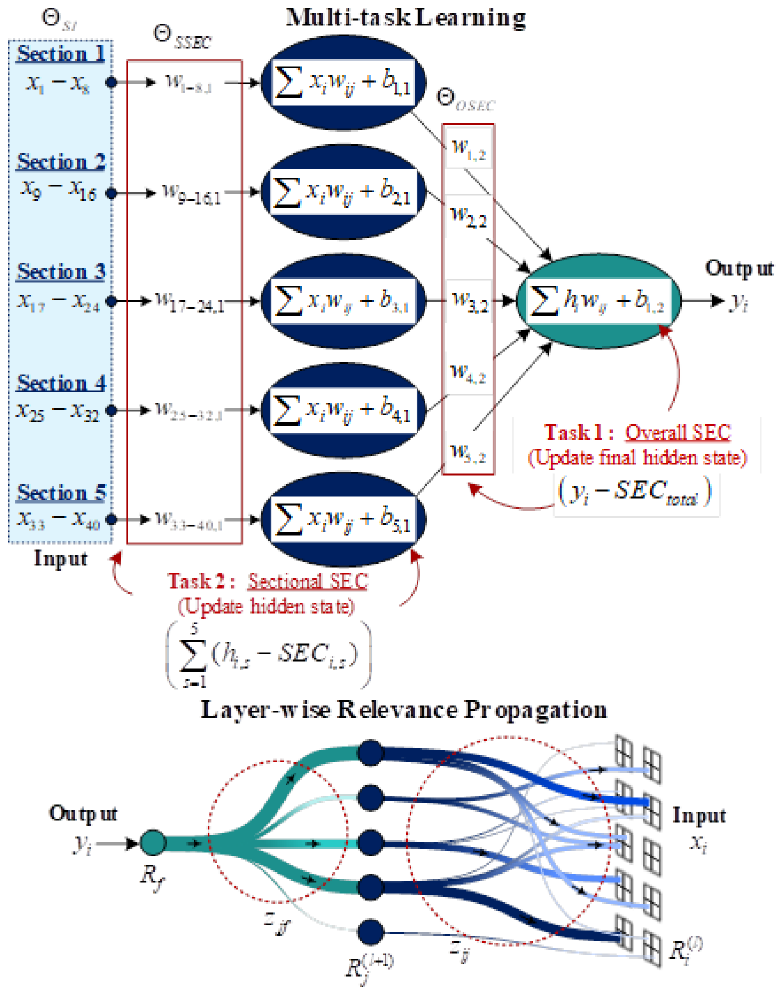
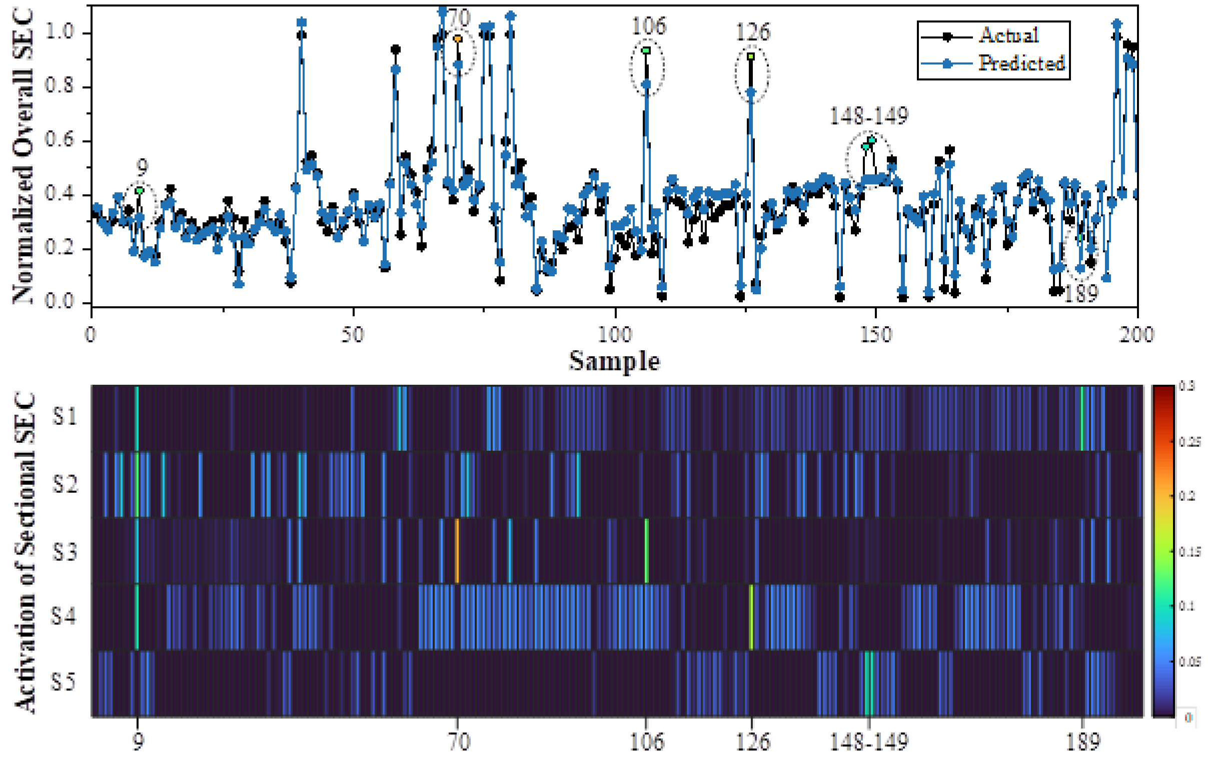


Fig.1 Network training and layer updating procedure of MTL-LRP

Energy efficiency gap



Direct Chlorination Section			Oxychlorination Section			EDC Purification Section			EDC Cracking Section			VCM Purification Section		
No.	Tag ID	Description	No.	Tag ID	Description	No.	Tag ID	Description	No.	Tag ID	Description	No.	Tag ID	Description
1	L-101	Ethylene feed rate	9	L-201	Oxygen feed rate	17	L-303	Inlet temperature T-301	25	L-401	Purified EDC mass flow	33	L-501	Inlet flow T-501
2	L-102	Chlorine feed rate	10	L-202	Ethylene feed rate	18	L-304	Temperature at Top T-301	26	L-401	Temperature of inlet F-401	34	L-503	T-501 top temperature
3	L-104	Outlet flow R-101	11	L-214	Outlet flow E-203	19	L-310	Inlet flow T-302	27	L-402	Fuel feed rate	35	L-507	T-501 bot temperature
4	L-105	Vent gas rate R-101	12	L-218	Inlet flow T-201	20	L-314	Inlet flow E-306	28	L-404	Temperature of cracked gas	36	L-513	VCM rate
5	L-106	EDC mass flow	13	L-229	Recycled HCl rate	21	Utility	CW mass flow E-301	29	L-424	Temperature recycled D-404	37	L-516	Recycled EDC rate
6	L-106	Temperature of EDC	14	L-229	Temperature of recycled HCl	22	Utility	CW mass flow E-304	30	Utility	CW mass flow E-401	38	Utility	LP steam rate E-502
7	Utility	Quench air R-101	15	Utility	CW mass flow E-204	23	Utility	LP rate E-303	31	Utility	CW mass flow E-402	39	Utility	CW mass flow E-503
8	Utility	LP rate E-101	16	Utility	LP rate E-205	24	Utility	LP rate E-305	32	Utility	CW mass flow E-403	40	Utility	MP steam rate E-504

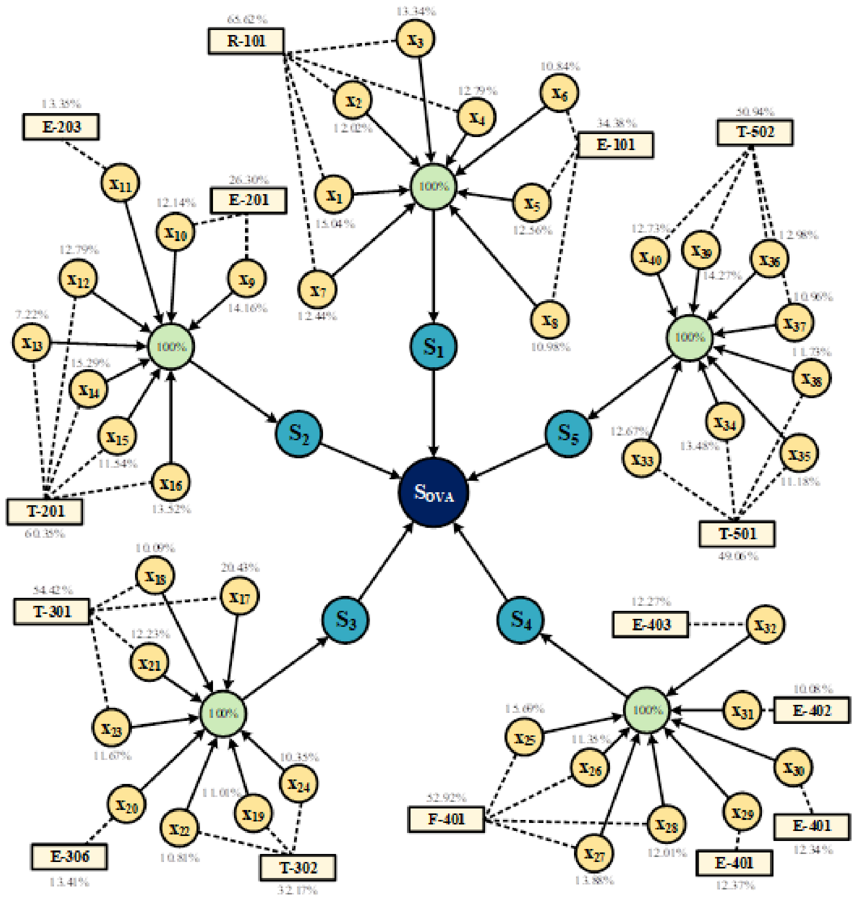
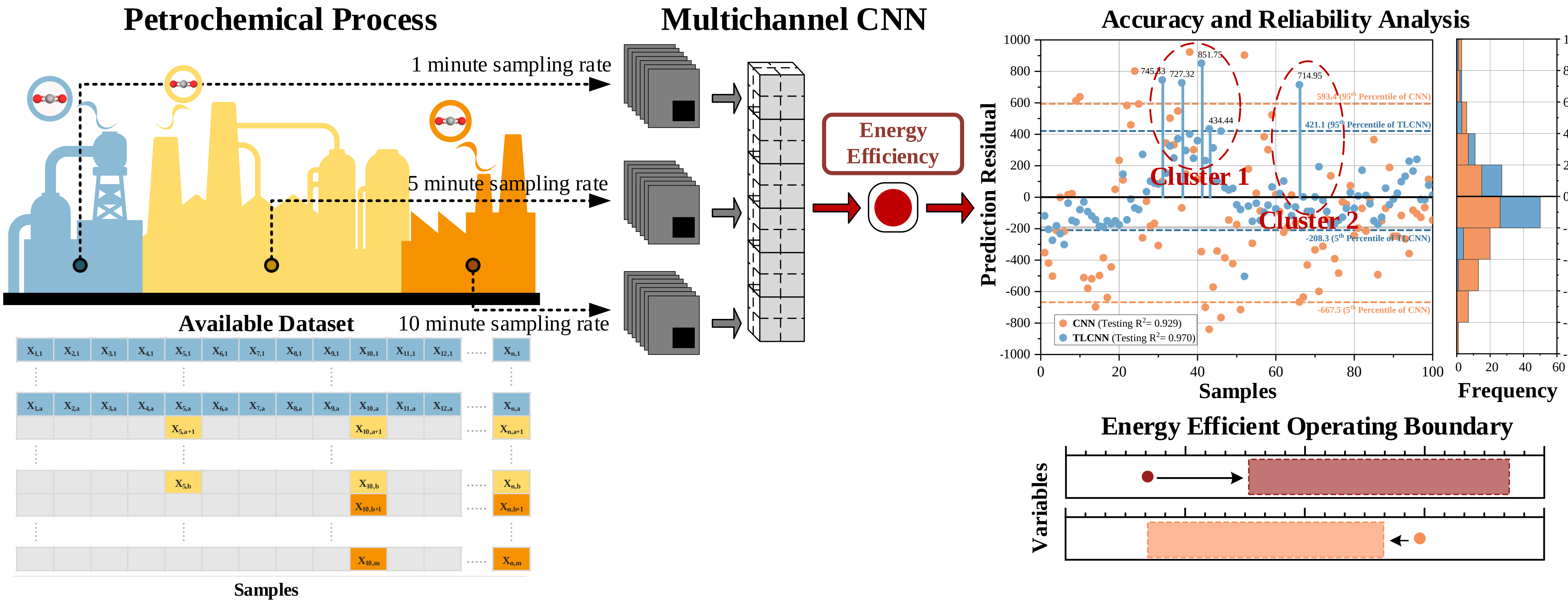


Fig.2 Contribution of the input weight to sectional and overall SEC on the system

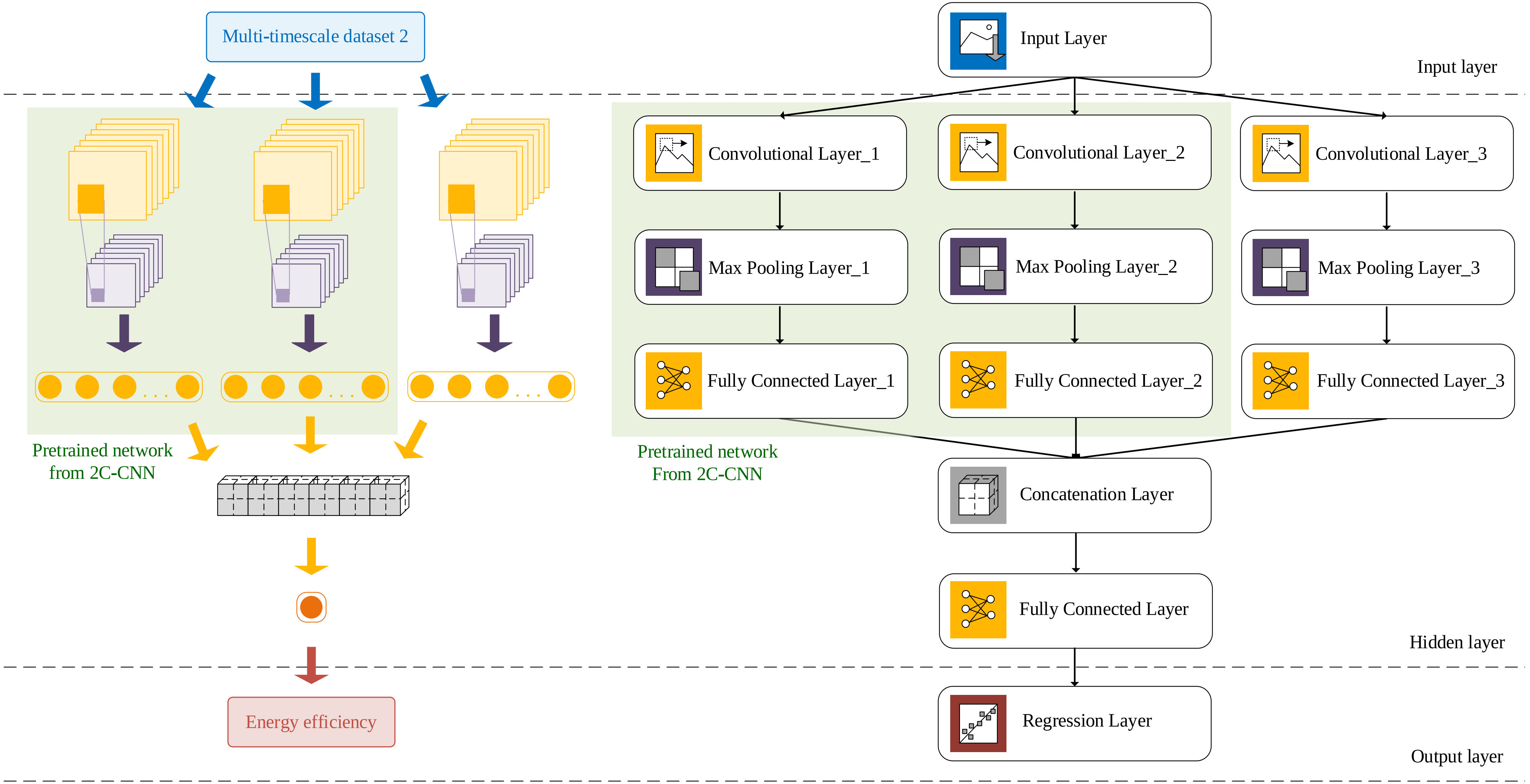
Energy efficiency analysis: multirate sampling process

Energy efficiency analysis for multirate sampling

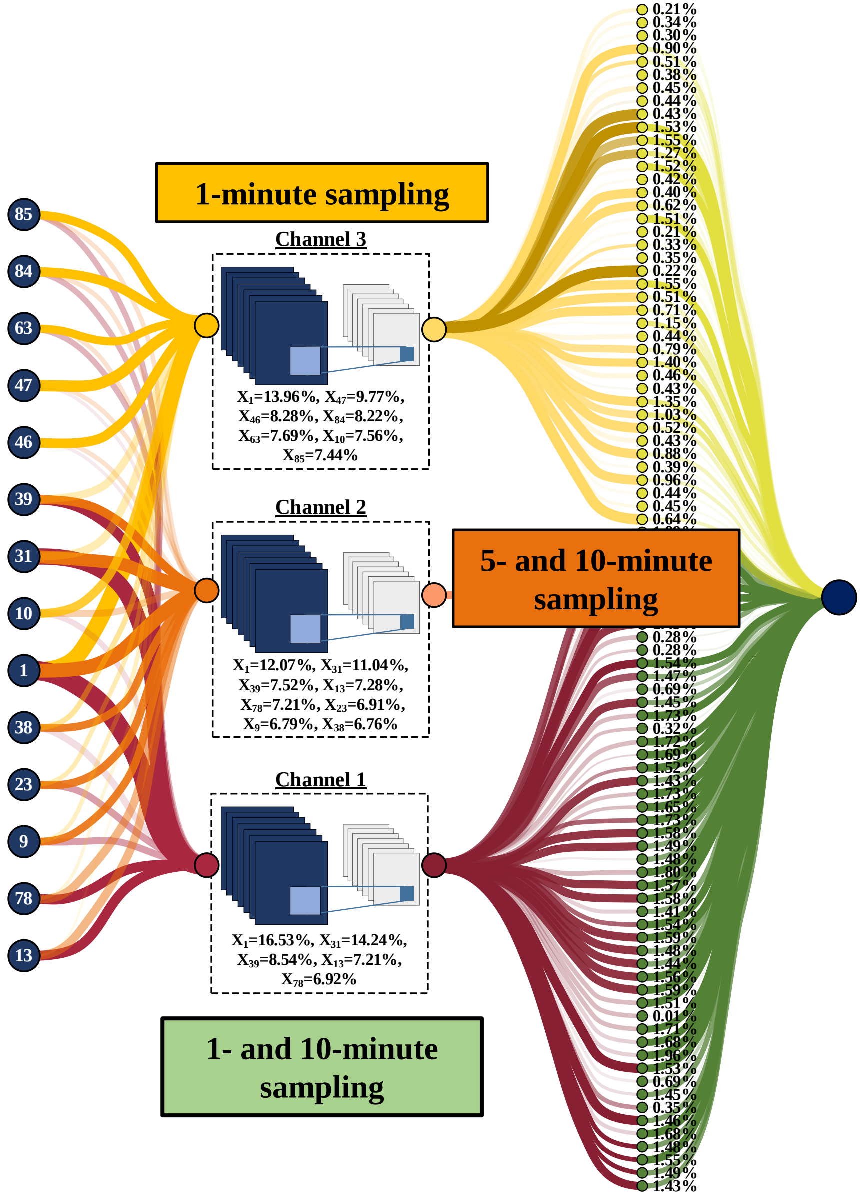


Panjapornpon C. Bardeeniz S., Hussain M.A., Vongvirat K, Chuay-ock C. “Energy efficiency and savings analysis with multirate sampling for petrochemical process using convolutional neural network-based transfer learning.” *Energy and AI* ,2023, 14: 100258.

Multichannel convolutional neural network



Model focus and reproducibility



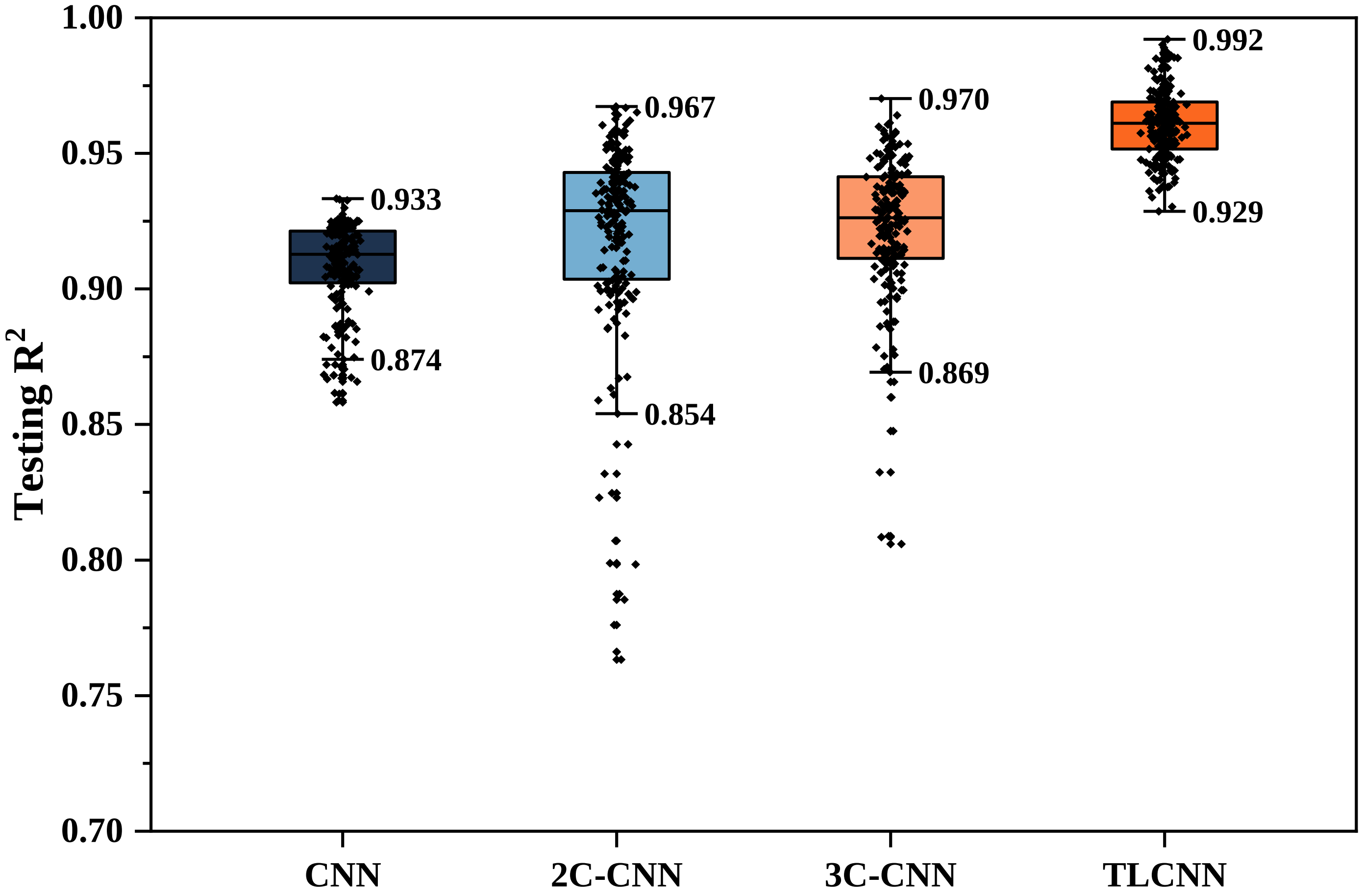


Fig. 3 Boxplot of testing R^2 values of CNN models.

Energy efficiency optimization

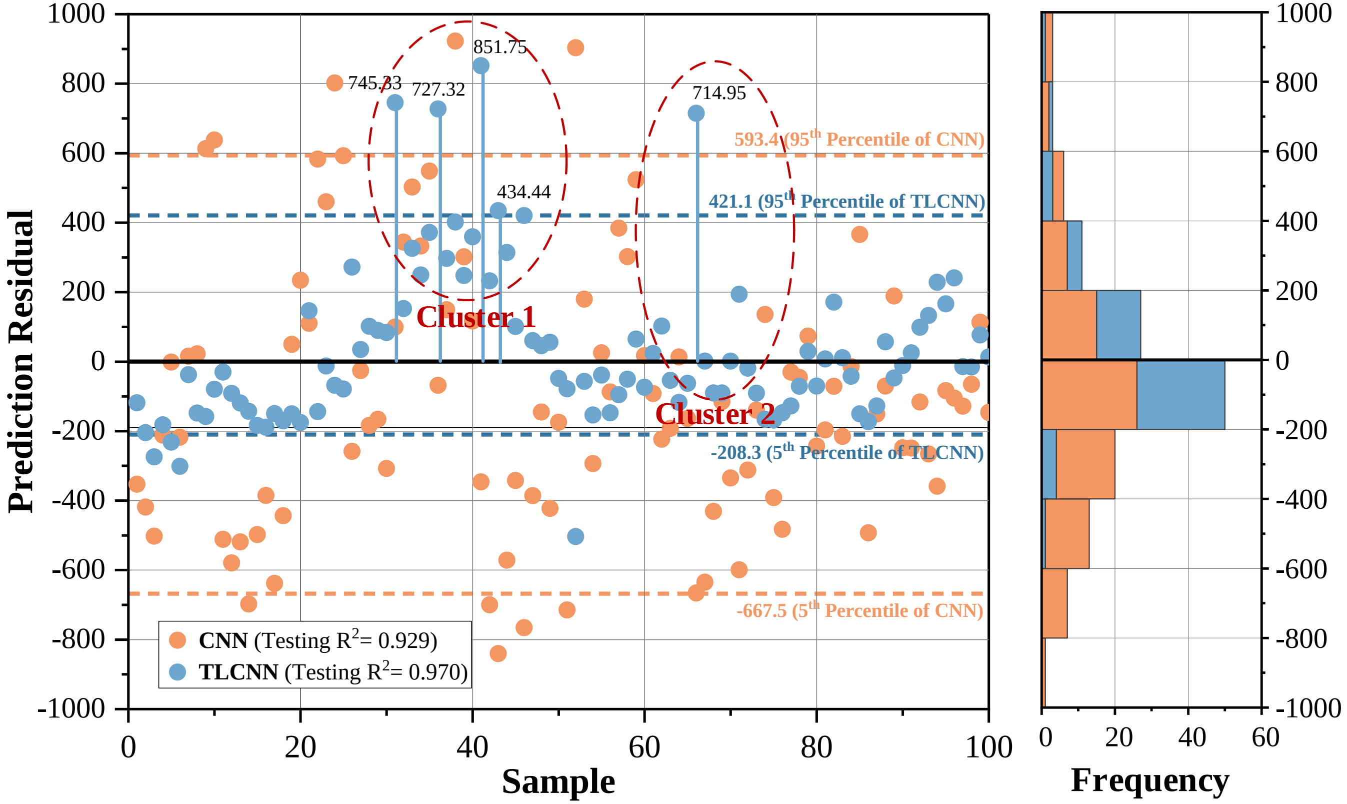


Fig.4 Residual plot of actual and benchmark SEC provided by models.

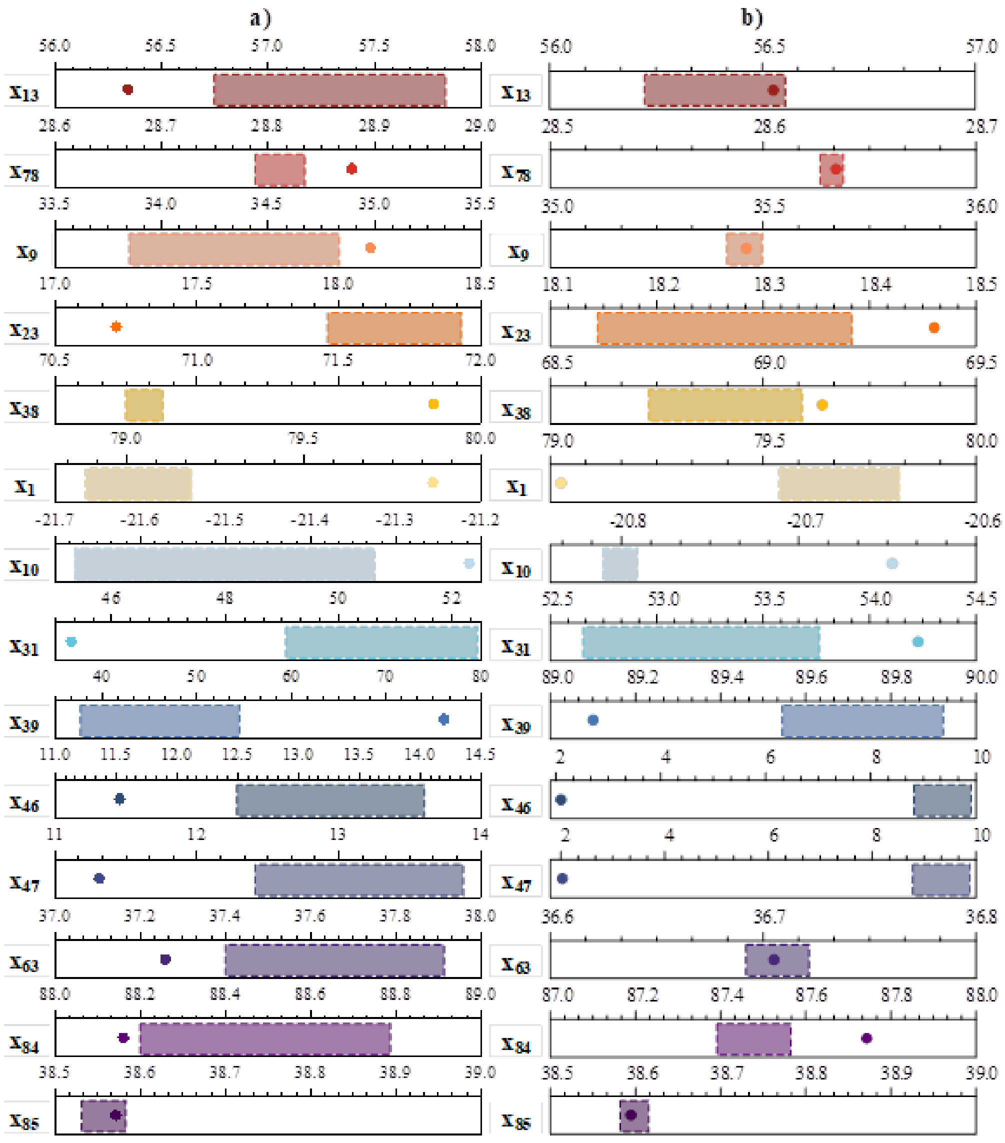
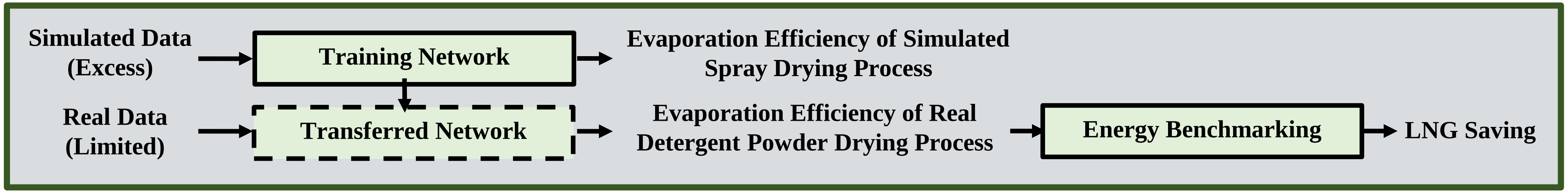
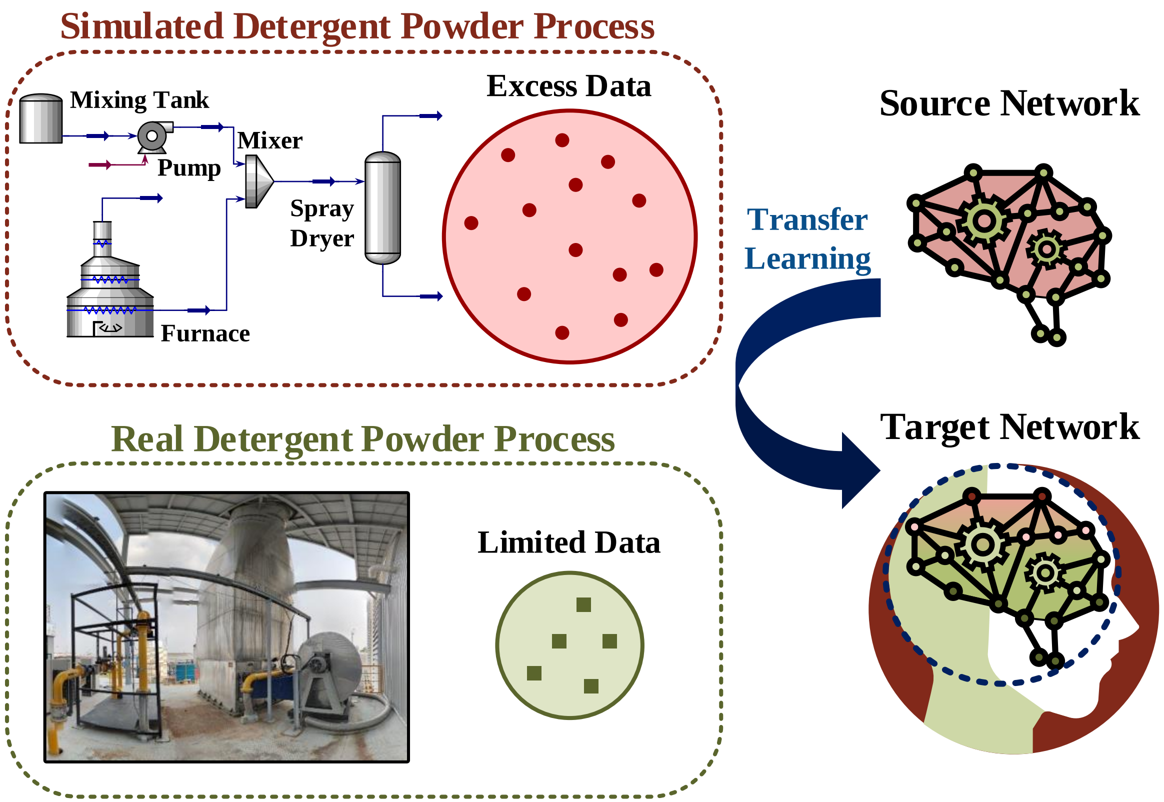


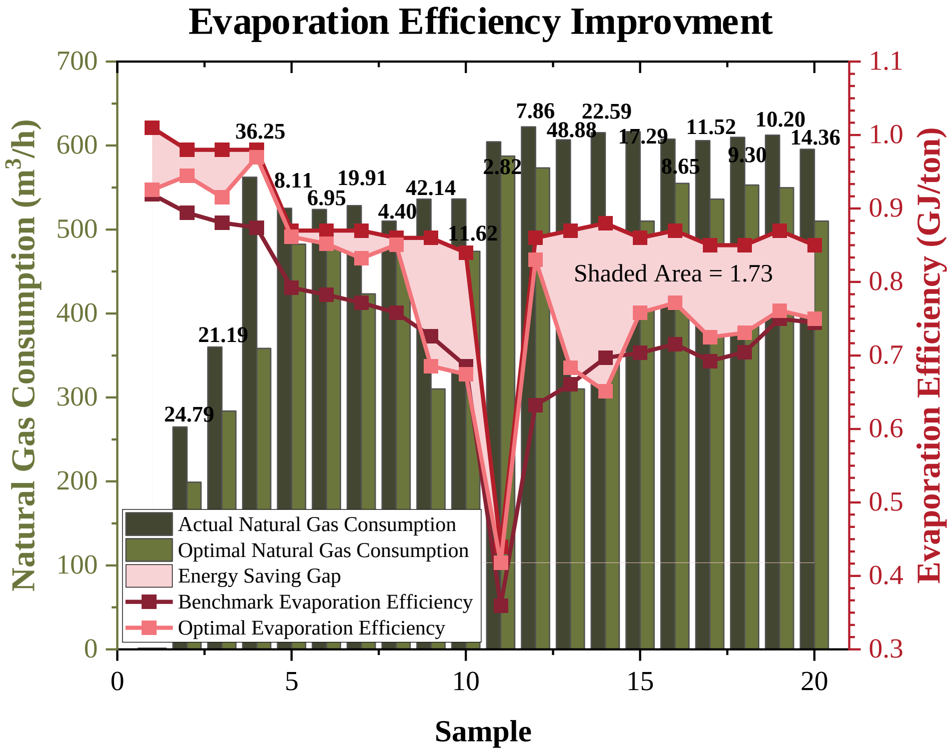
Fig.5 Benchmarking of energy efficient operating range

Energy efficiency analysis: under limited data

Energy efficiency prediction through digital twin aided model







Bardeeniz S., Panjapornpon C., Fongsamut C., Ngaotrakanwiat P., Hussain M.A. Digital twin-aided transfer learning for energy efficiency optimization of thermal spray dryers: leveraging shared drying characteristics across chemicals with limited data. Applied Thermal Engineering. 2024; 242, 122431.

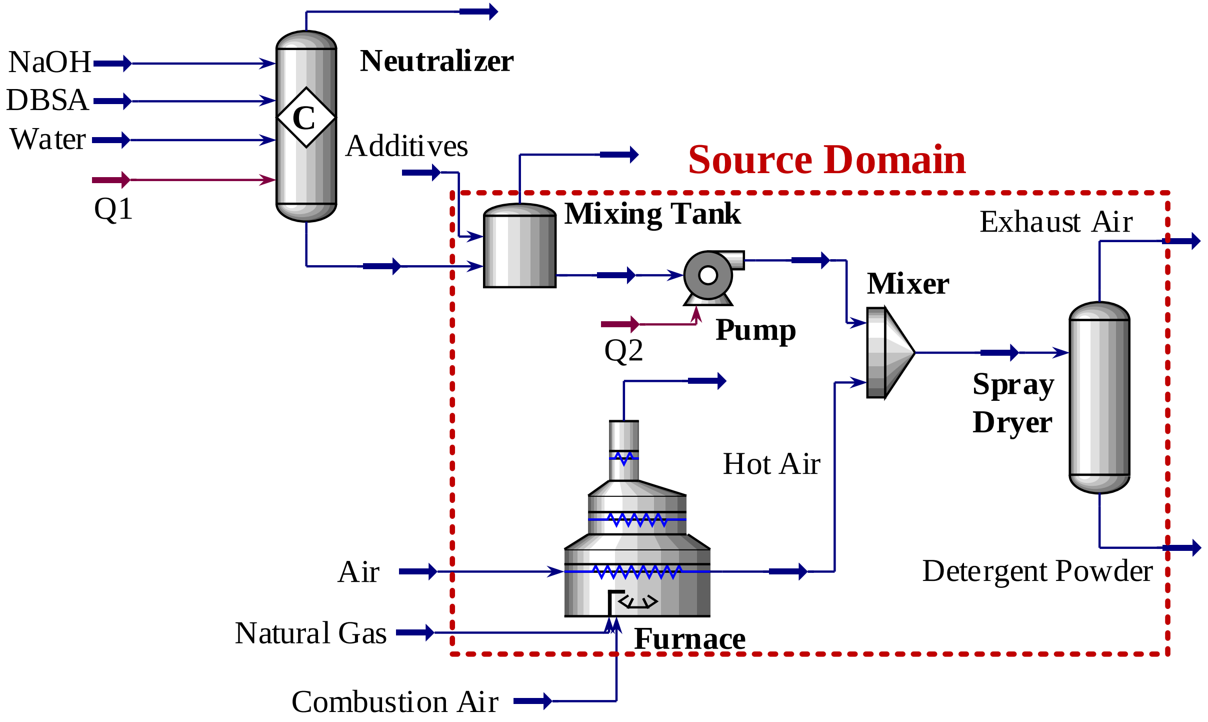
Digital twin aided transfer learning concept

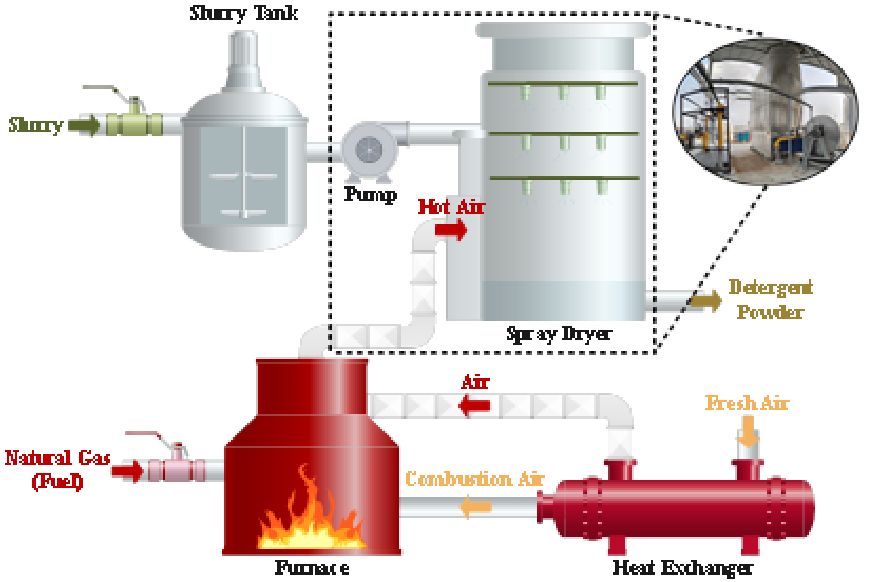
Small Scale Simulation → **Large Scale Operation**

Shared Knowledge

Different Product and Scale

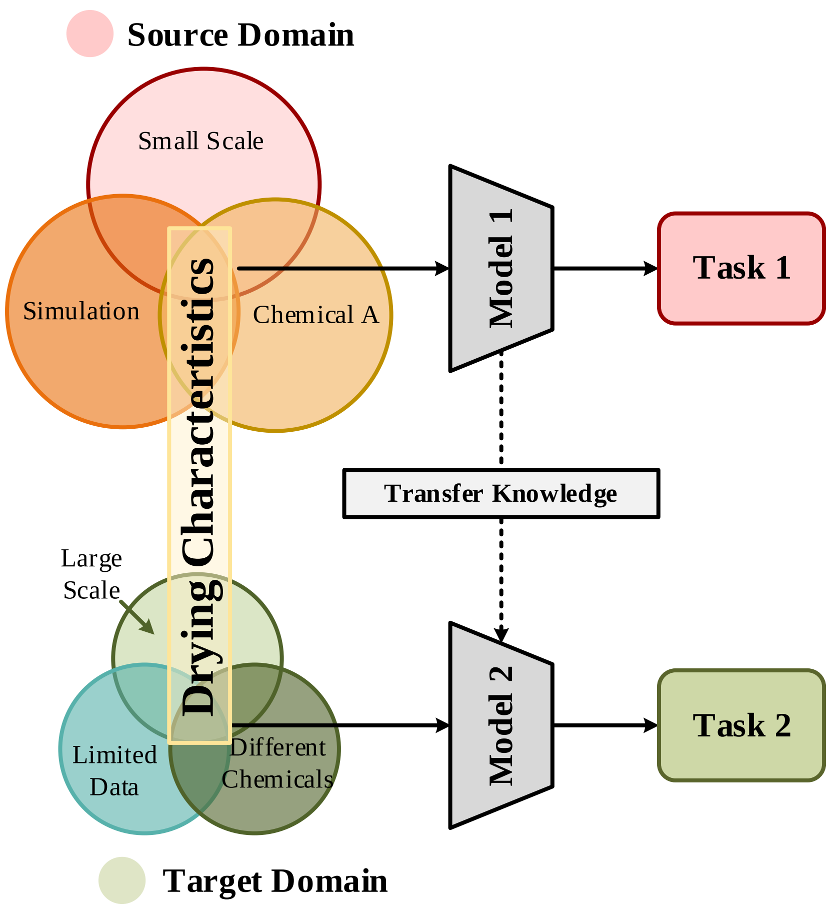
Same Characteristics





Input Variables	
No.	**Description**
1	Temperature of slurry
2	Moisture content of base powder
3	Spray dryer feed rate
4	Temperature of exhaust air
5	Ambient temperature
6	Drying pressure
7	Natural gas feed rate
Output Variable	
No.	**Description**
8	Evaporation efficiency

Digital twin aided transfer learning concept



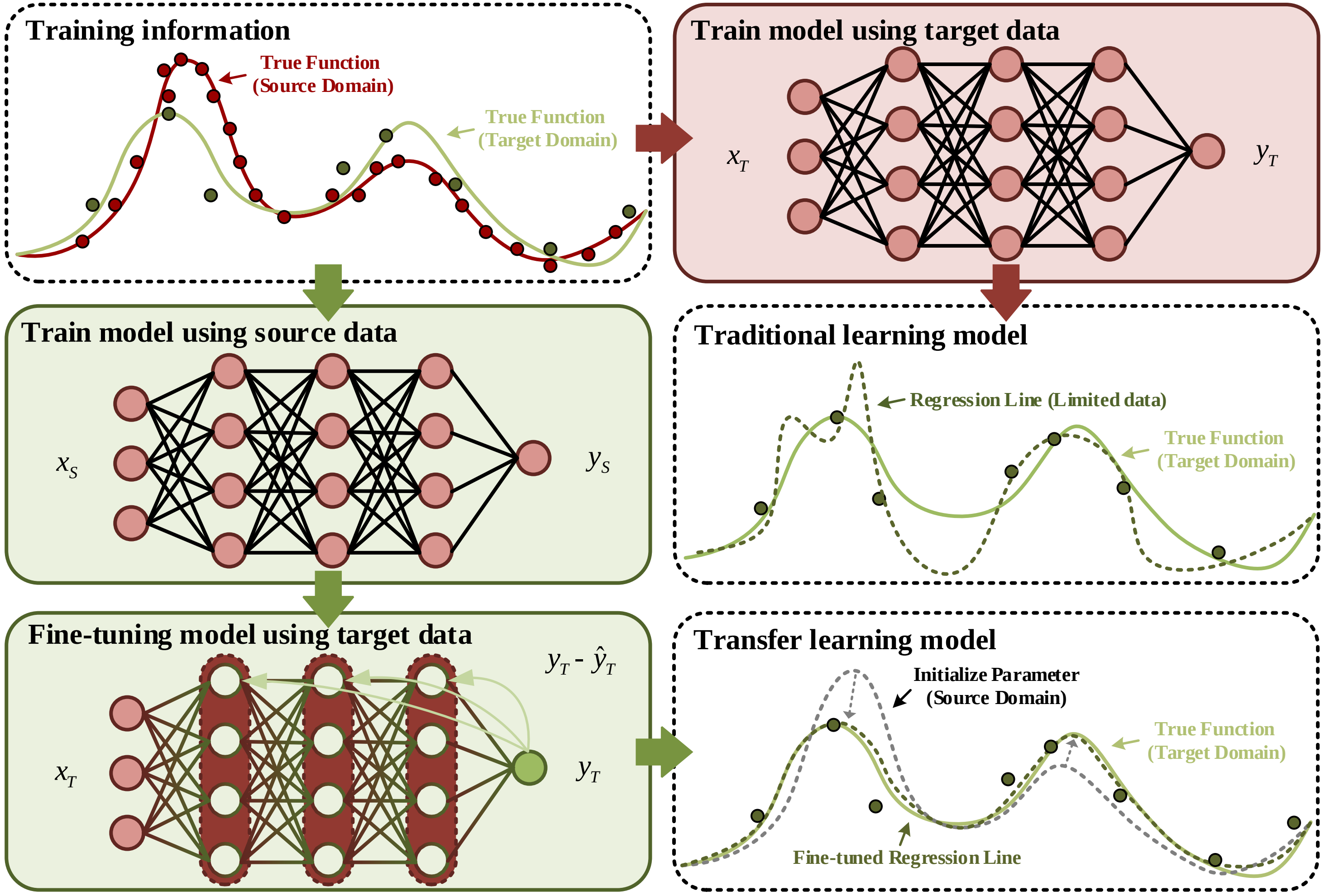


Fig.6 Comparison of prediction plane networks trained using traditional and transfer learning.

Energy efficiency prediction result

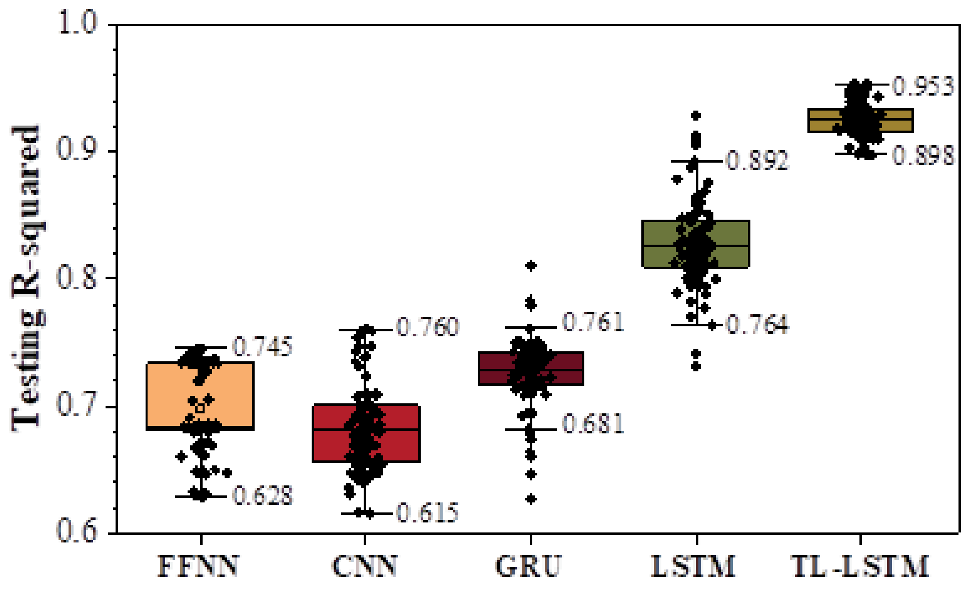


Fig.7 Reliability analysis results of deep learning model.

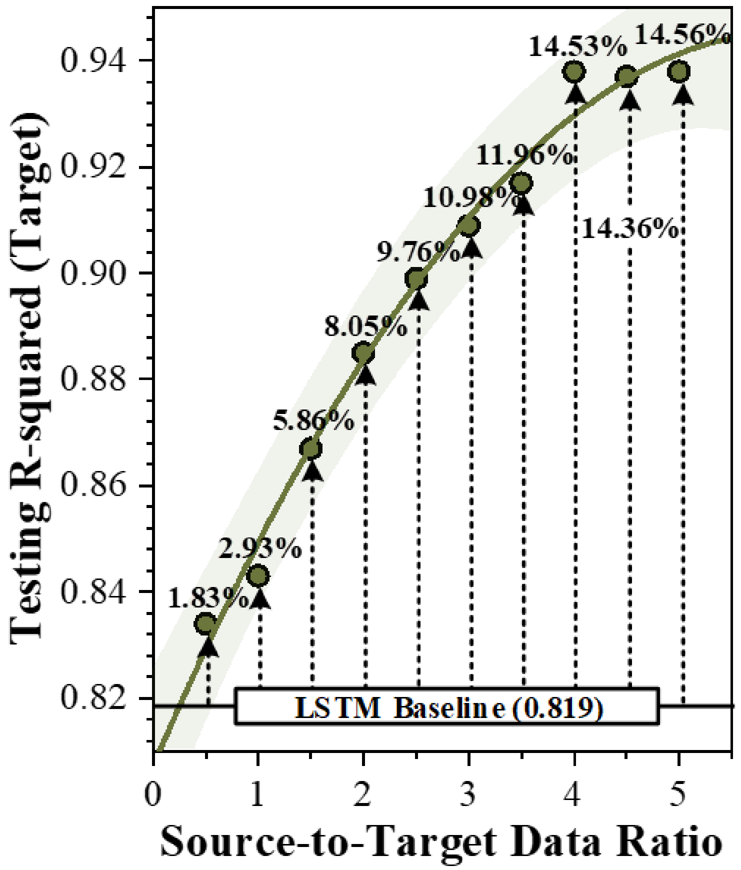


Fig.8 Effect of source domain on testing r-squared of target domain.

Energy efficiency prediction result

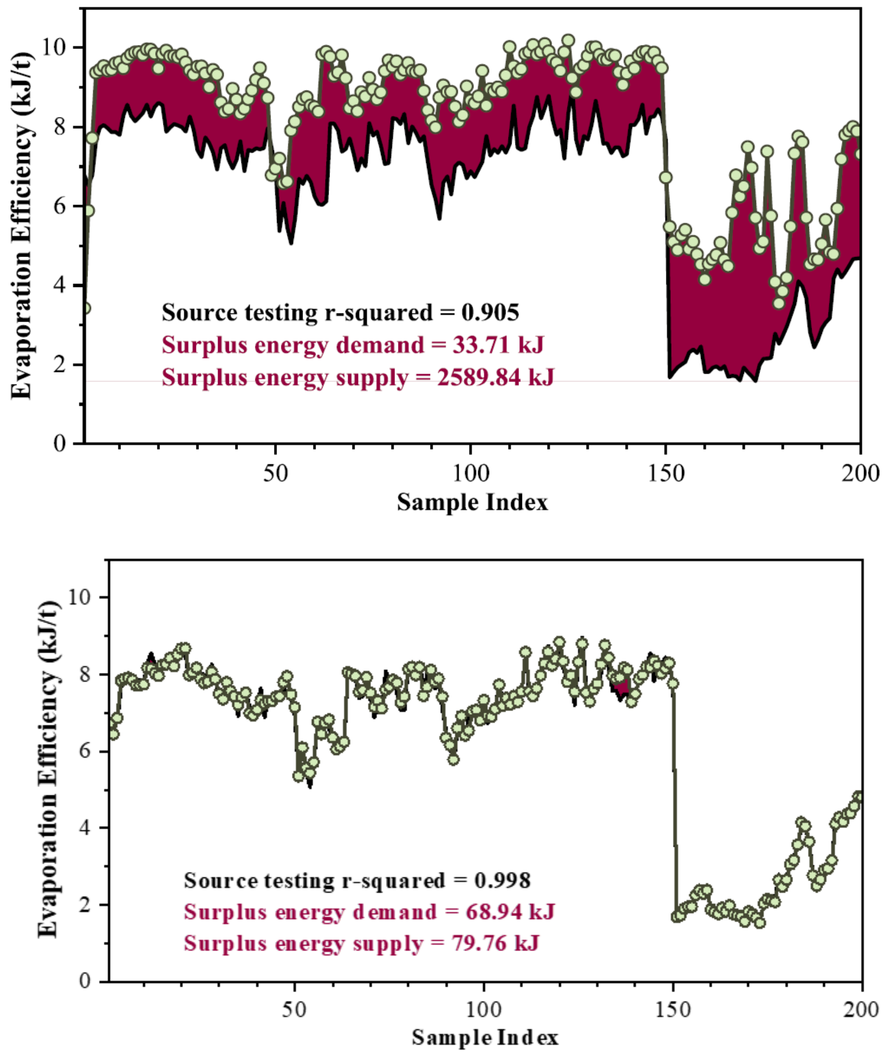


Fig.9 Surplus energy demand and supply in the source domain for different options of source accuracy.

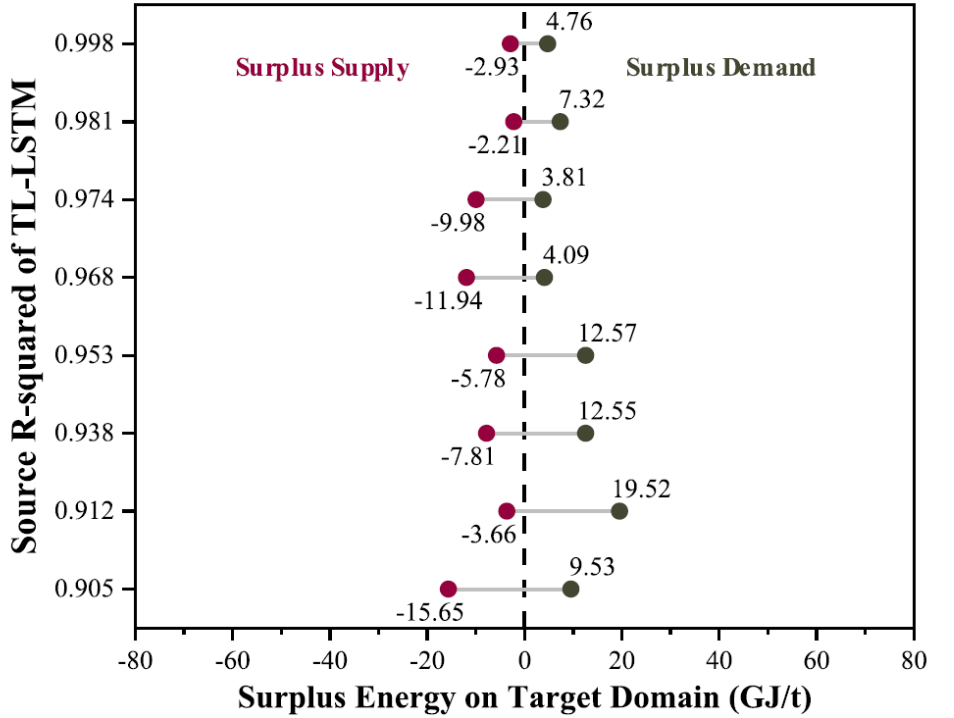
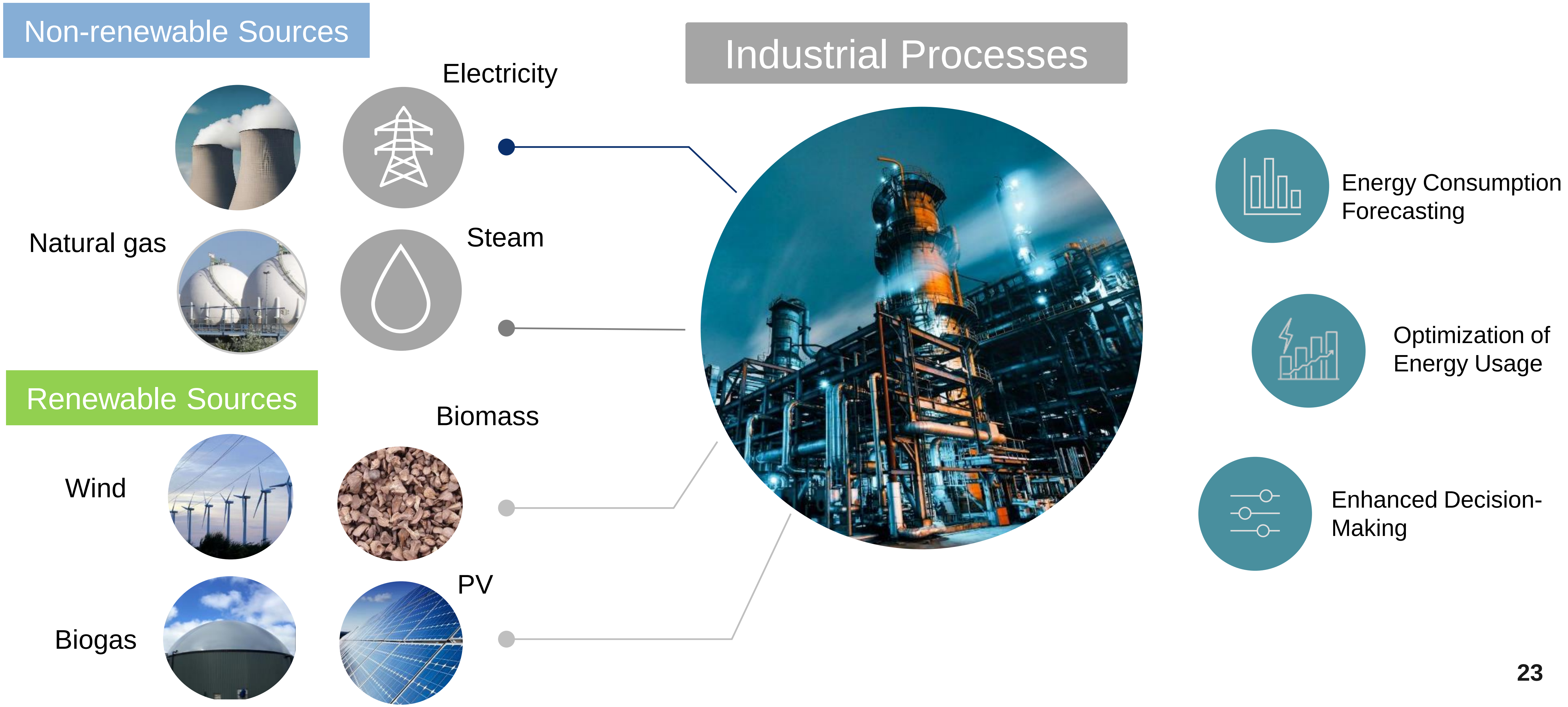


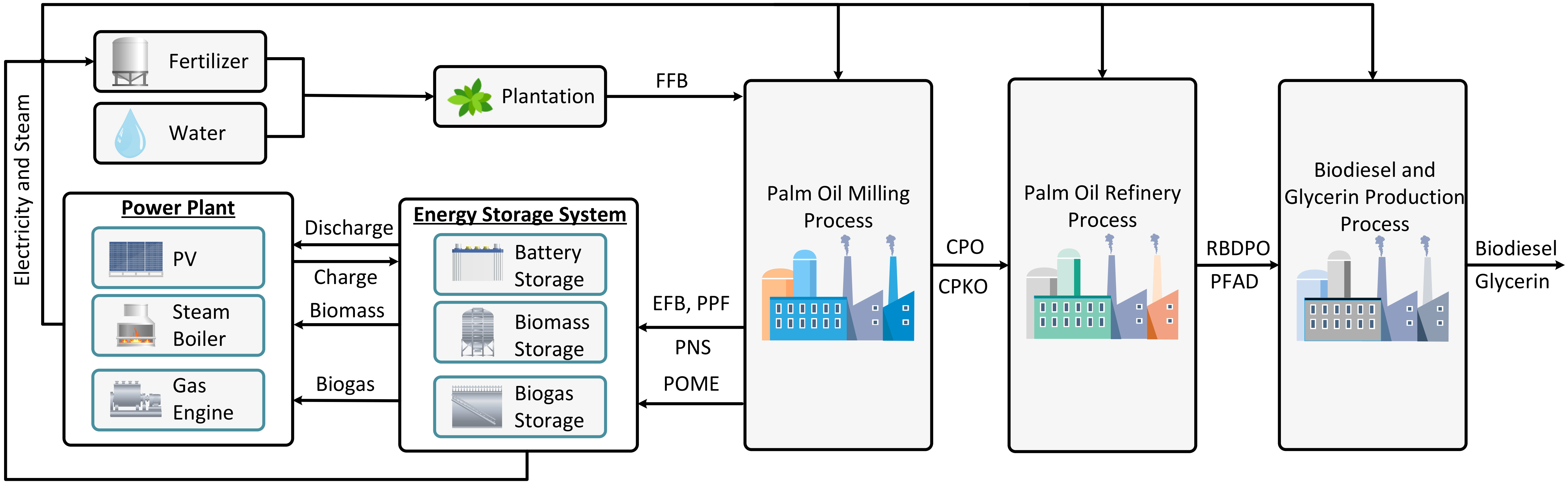
Fig.10 Surplus energy demand and supply comparison using different source networks.

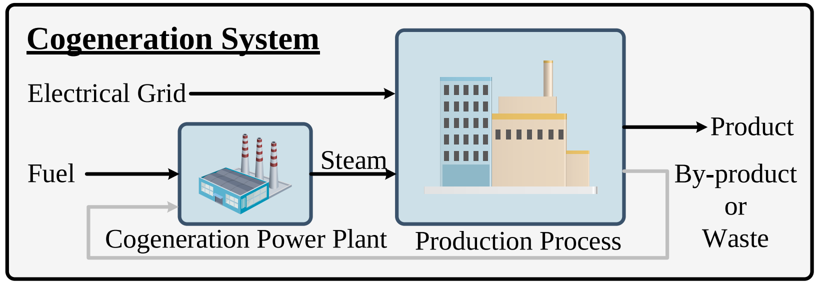
Decision of energy optimization

Energy management for industrial processes



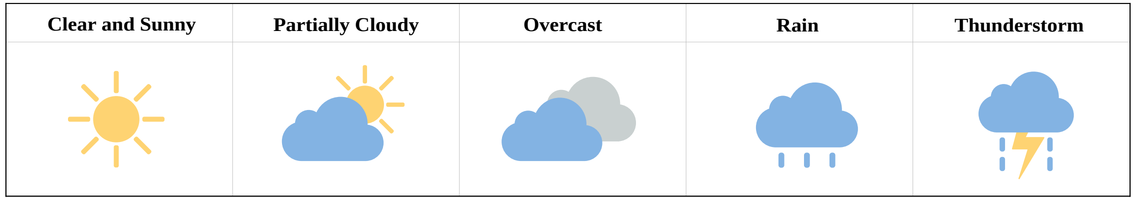
Case study: Complex of palm oil industry

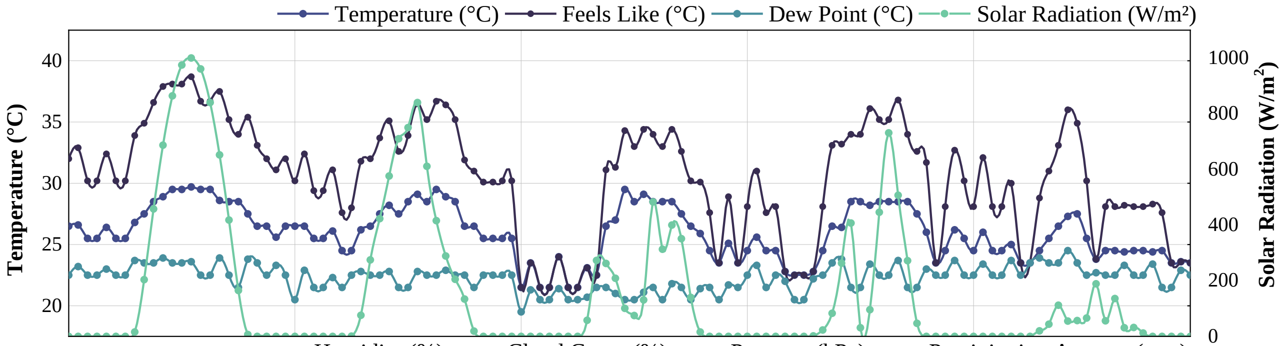


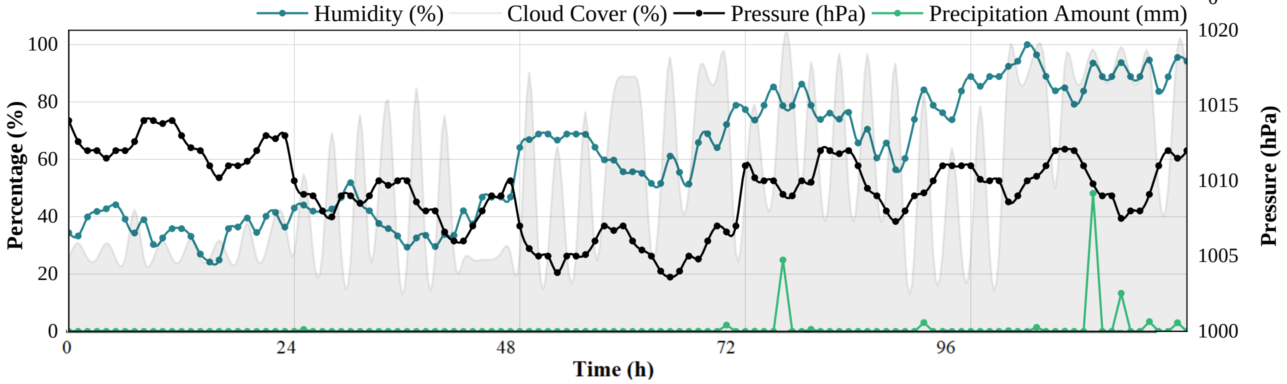


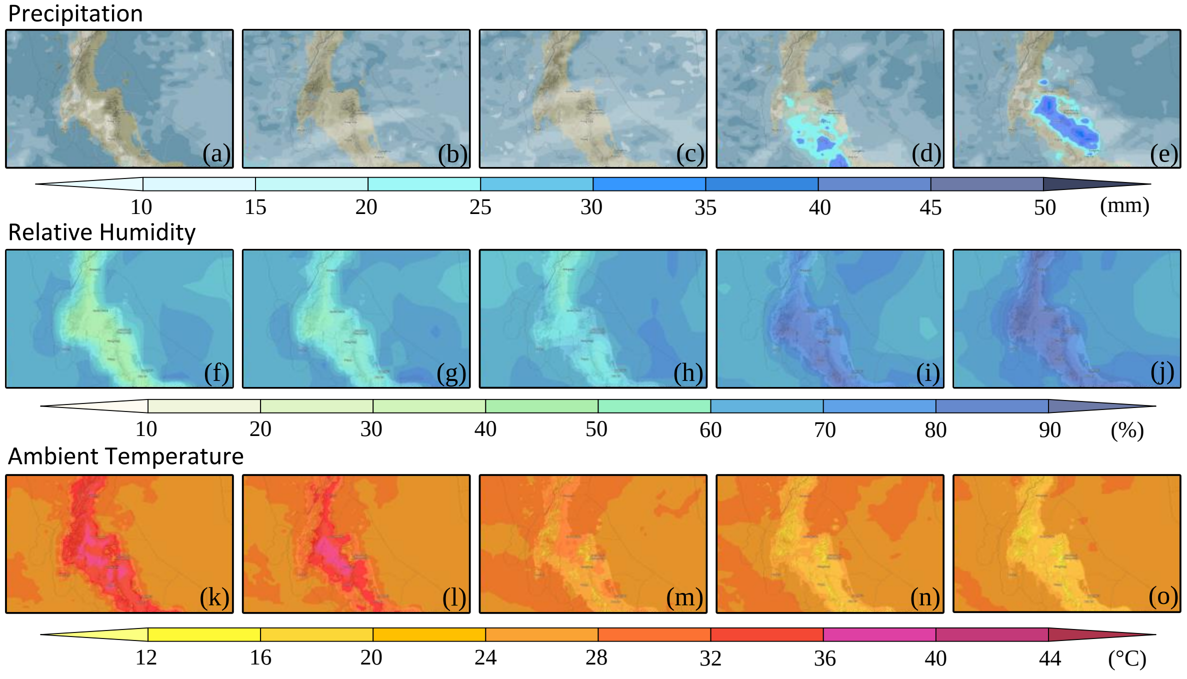
Zero Waste

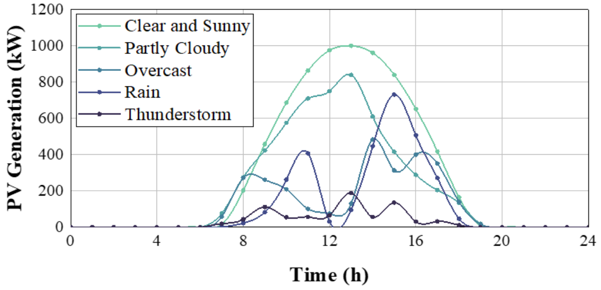
Impact of climatic variability

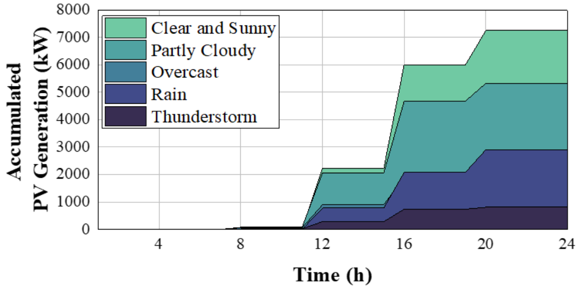




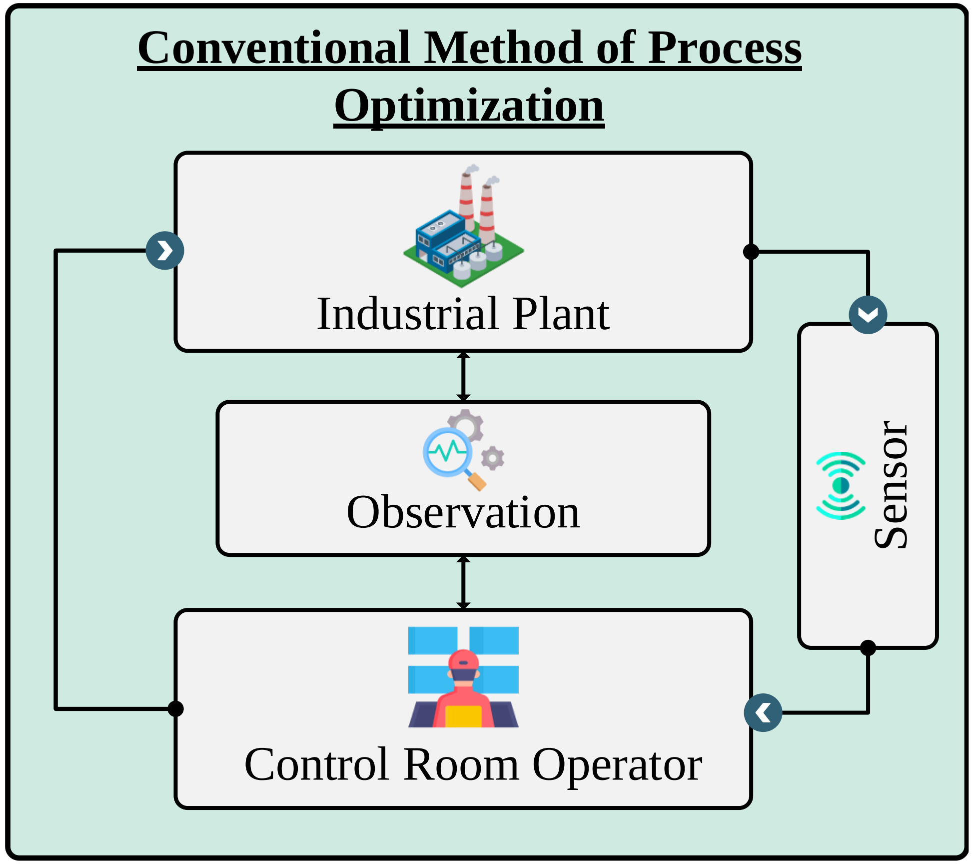


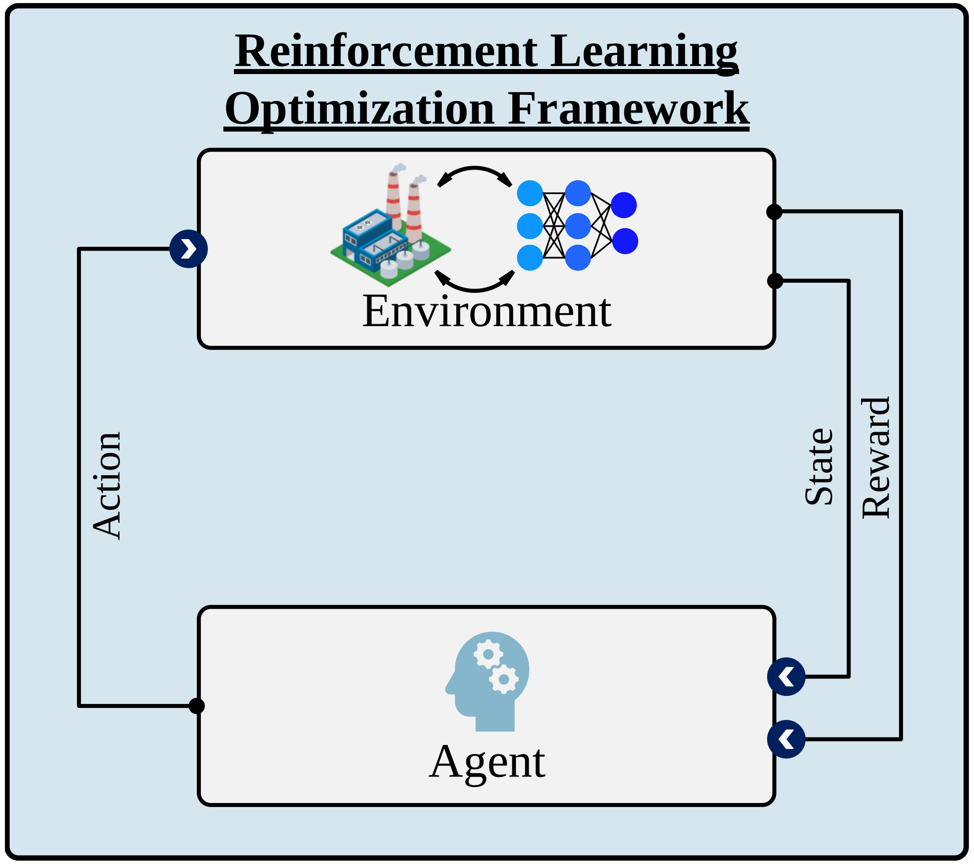






Reinforcement learning (RL) optimization



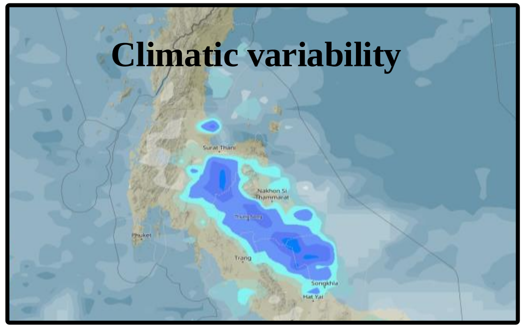


Energy management with RL

Inputs → Methods → Outputs

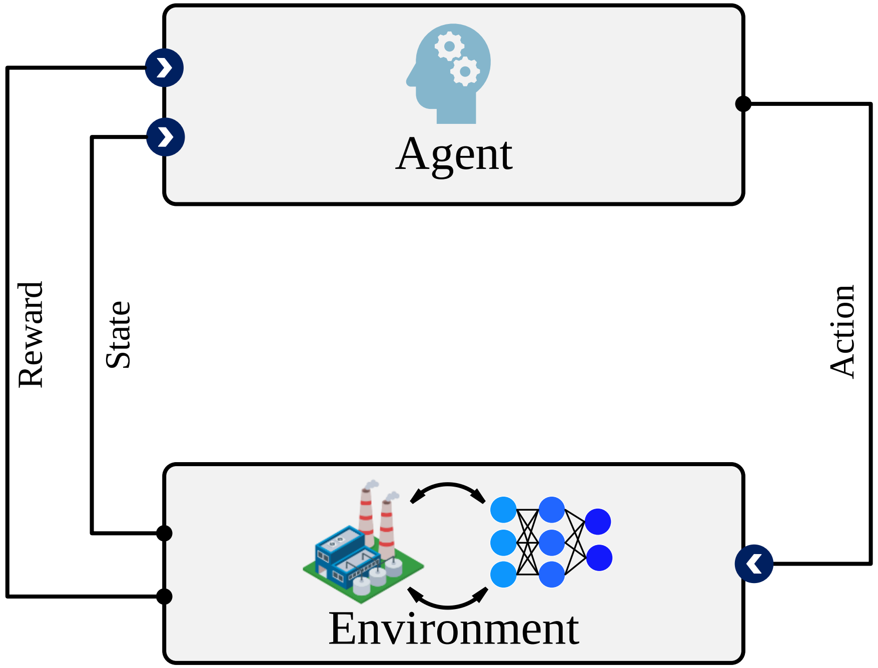
Input data

- Ambient temperature (°C)
- Relative humidity (%)
- Electricity consumption (MW)
- Steam consumption (t/h)
- Biomass storage (t)
- Biogas storage (m^3)
- PV battery storage (kW)

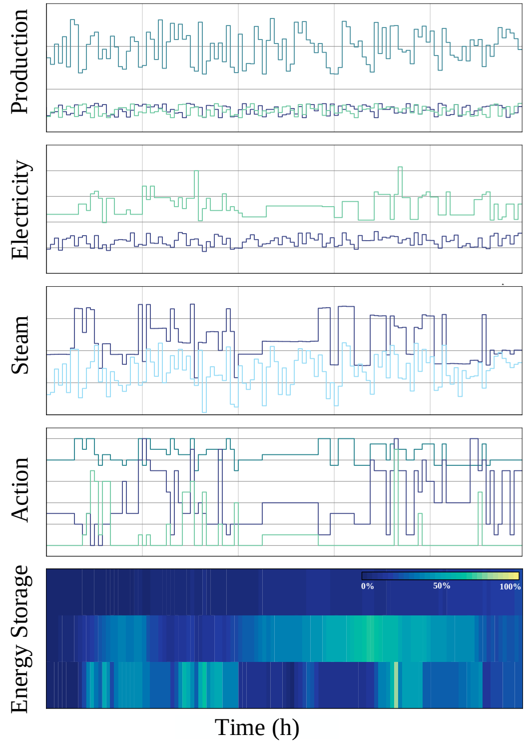


DQN Model

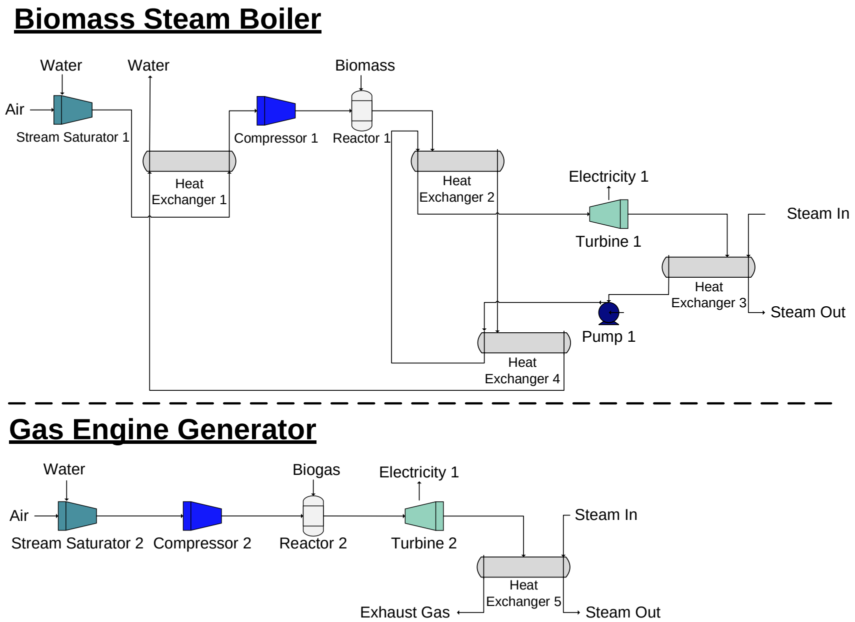
$$Q(s_t,a_t) = Q(s_t,a_t) + \alpha[R_{t+1} + \gamma \max_a Q(s_{t+1},a') - Q(s_t,a_t)]$$



Energy management results



Environment model



Environment

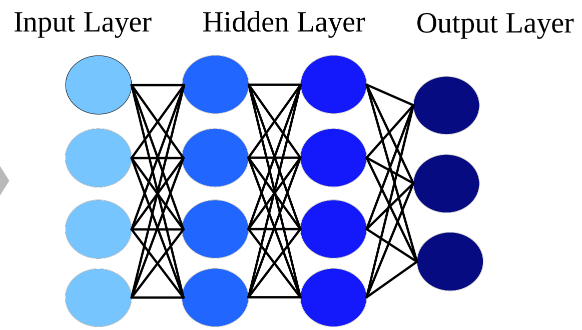


Table 2 Input and output variables for the environment model

Power plant	Input variable	Output variable
Biomass steam boiler	X1 Ambient temperature (^oC)	Y1 Biomass mass flow (kg/h)
	X2 Relative humidity (%)	Y2 Steam output (kg/h)
	X3 Power output steam boiler (kW)	Y3 CO_2 emissions (kg/h)
Gas engine generator	X1 Ambient temperature (^oC)	Y1 Biogas mass flow (kg/h)
	X2 Relative humidity (%)	Y2 Steam output (kg/h)
	X3 Power output generator (kW)	Y3 CO_2 emissions (kg/h)

Reinforcement Learning

Reward

$$R = \begin{cases} if\ S_{bm}^{lb} < S_{bm} < S_{bm}^{ub}\ and\ S_{bg}^{lb} < S_{bg} < S_{bg}^{ub}\ and\ S_{PV}^{lb} < S_{PV} < S_{PV}^{ub} \\ \quad R = -EDR - SDR - SER \\ else \\ \quad R = -1{,}000 \end{cases}$$

$S = \text{Storage},\ bm = \text{Biomass},\ bg = \text{Biogas}$

Electricity Demand Reward: $EDR = k_1 \cdot \max(0, P_d - (P_{bm} + P_{bg} + P_{PV}))$

Steam Demand Reward: $SDR = k_2 \cdot \max(0, ST_d - (ST_{bm} + ST_{bg}))$

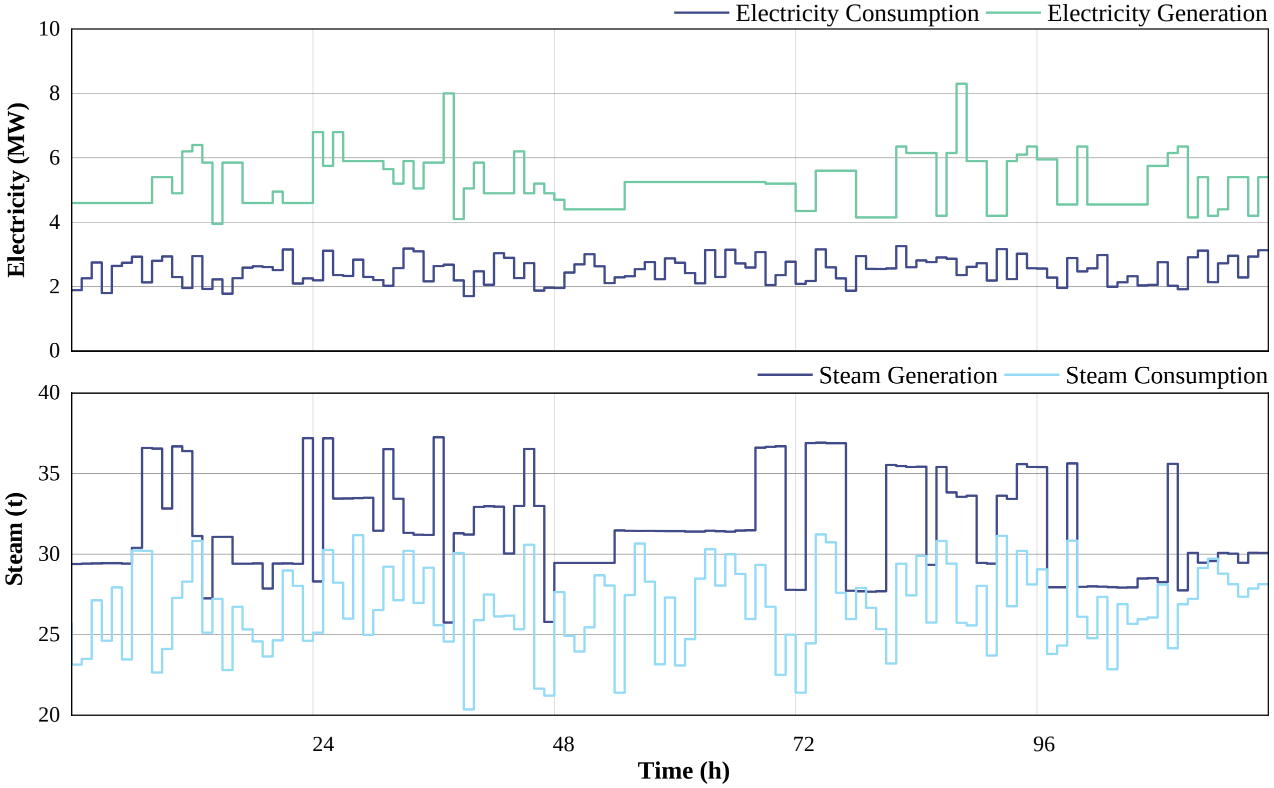
Sustainability Energy Reward: $SER = (k_3 \cdot P_{bm}) + (k_4 \cdot P_{bg}) + (k_5 \cdot P_{PV})$

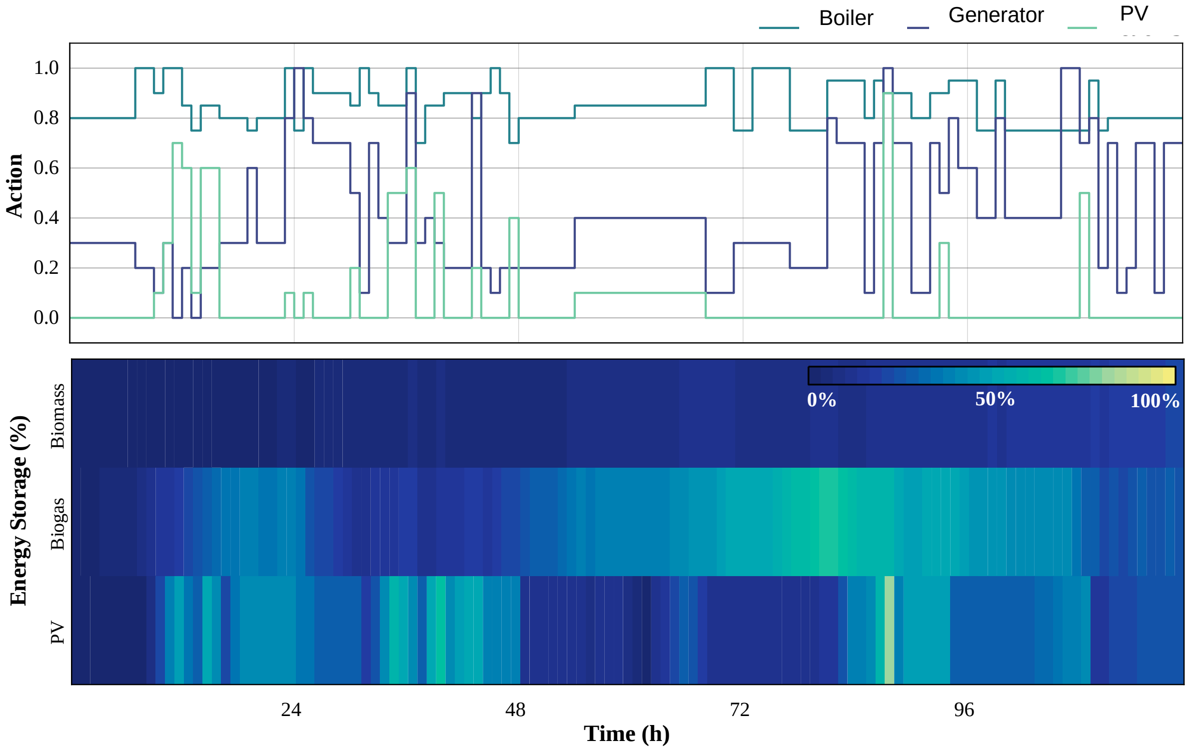
State and Action

Table 3 List of input and output variables for the environment model.

Element	Variable	Range	Domain
Action	Capacity of the Biomass Steam Boiler (%)	[0, 100] + 5%	Discrete
	Capacity of the Gas engine generator (%)	[0, 100] + 10%	Discrete
	Capacity of the PV battery storage (%)	[0, 100] + 10%	Discrete
State	Ambient temperature (ºC)	[0, 40]	Continuous
	Relative humidity (%)	[0, 100]	Continuous
	Electricity consumption (MW)	[0, 10]	Continuous
	Steam consumption (t/h)	[0, 52]	Continuous
	Biomass storage (t)	[0, 500]	Continuous
	Biogas storage (m^3)	[0, 10,000]	Continuous
	PV battery storage (kW)	[0, 3000]	Continuous

Energy management under climatic variability result





Thank you