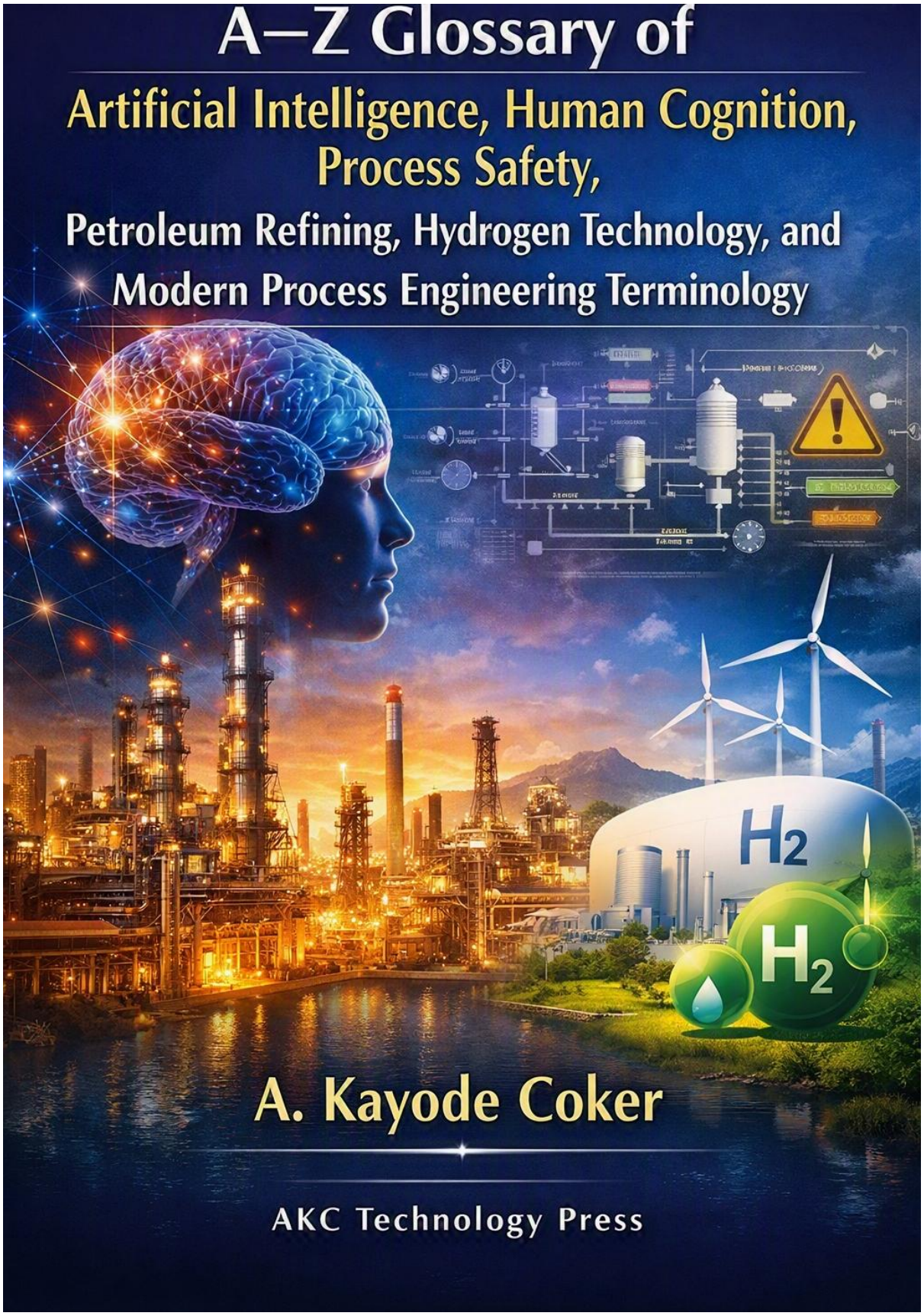

A–Z Glossary of
Artificial Intelligence, Human Cognition, Process Safety,
Petroleum Refining, Hydrogen Technology, and Modern Process Engineering Terminology
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A. Kayode Coker
AKC Technology Press



A–Z Glossary of Artificial Intelligence, Human Cognition, Process Safety, Petroleum Refining, Hydrogen Technology, and Modern Process Engineering Terminology

By

A. Kayode Coker

AKC Technology Press

Glossary

A

Abnormal-Condition Detection: The use of statistical methods, process monitoring, AI, or machine learning to identify operating behaviour that differs from established normal conditions.

Example: Detecting an unusual reactor-temperature rise before it develops into a runaway reaction.

Accountability: The professional obligation to accept responsibility for engineering decisions and their consequences. AI may provide recommendations, but the engineer remains accountable for the final decision.

Activation Function: A mathematical function within an artificial neural network that determines the output of an artificial neuron. Activation functions enable neural networks to learn nonlinear relationships.

Advanced Process Control (APC): A group of control techniques used to improve process stability, product quality, energy efficiency, and profitability.

AI and ML may enhance APC by providing predictions and optimized operating targets.

AI-Enabled Alarm Management: The use of AI to analyse, prioritize, and interpret process alarms so that operators can focus on the most urgent and safety-critical conditions.

American Petroleum Institute (API): An industry organization that develops standards, recommended practices, equipment specifications, and technical guidance for petroleum and natural-gas operations.

American Petroleum Institute Gravity (API Gravity): A measure of the density of crude oil or petroleum products relative to water. It is normally expressed in degrees API, written as °API.

$$^{\circ}\text{API} = \frac{141.5}{\text{Sp.Gr}} - 131.5 \qquad (1)$$

A high API gravity indicates a lighter petroleum liquid, while a low API gravity indicates a heavier liquid.

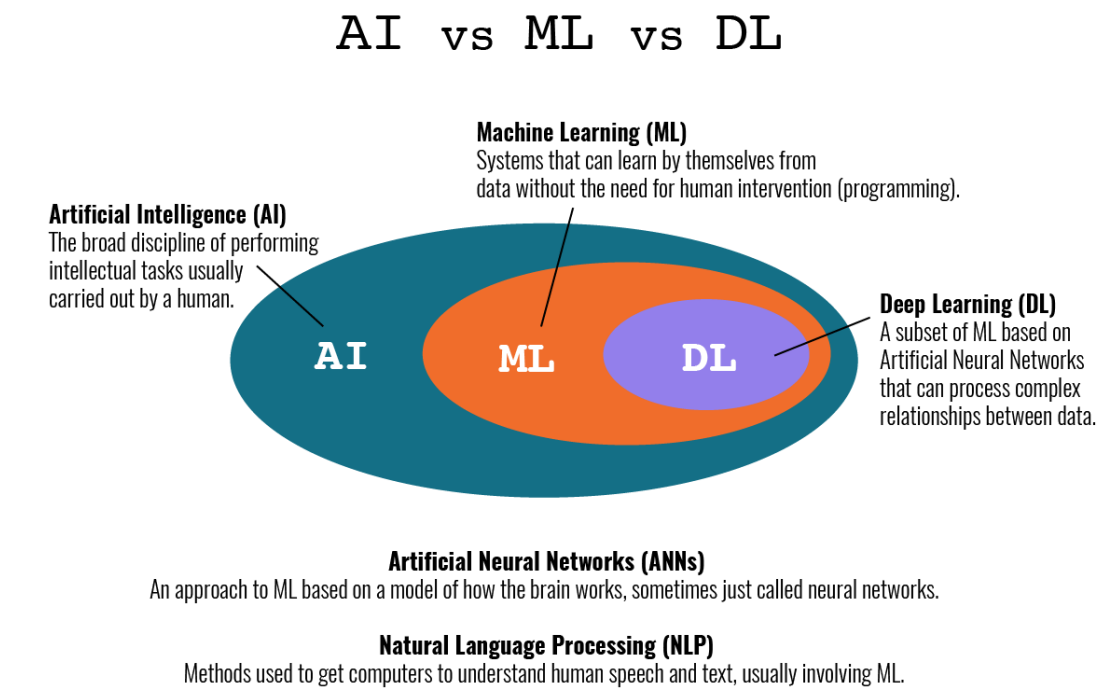
Example: A crude oil with an API gravity of 40°API is lighter than a crude oil with an API gravity of 22°API.

Anomaly Detection: The identification of unusual data patterns, equipment behaviour, or process conditions that may indicate a developing fault, sensor problem, or unsafe operation.

Example: An Autoencoder may identify an abnormal compressor-vibration pattern that differs from normal operating data.

Artificial: Something that is human-made, engineered, constructed, or synthesized rather than naturally occurring. In Artificial Intelligence, “artificial” does not mean false; it means engineered.

Artificial Intelligence (AI): The broad field concerned with developing computer systems that can perform functions associated with human intelligence, including learning, prediction, reasoning, diagnosis, optimization, language processing, and decision support.



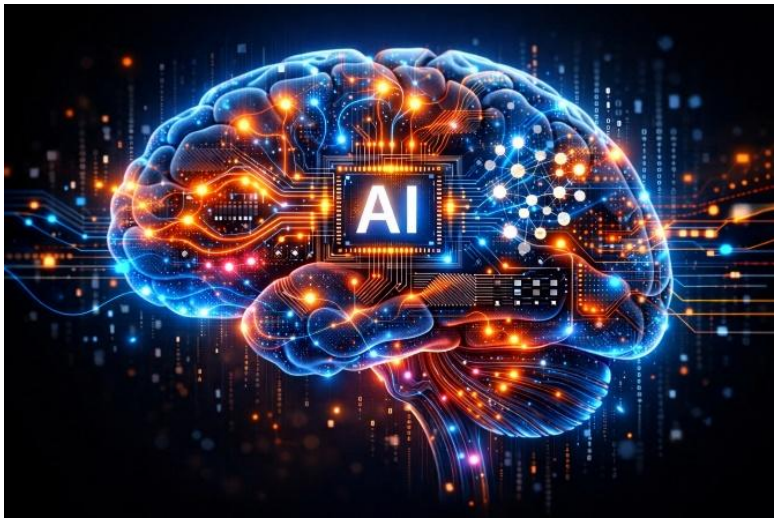


Figure 1. Cognitive human brain infused with AI and ML, glowing neural pathways, digital circuits and data streams integrated into the brain structure (Source: Author's illustrative visualization developed with AI-assisted tools.)

Artificial Neural Network (ANN): A machine-learning model composed of interconnected mathematical processing nodes inspired loosely by biological neurons. ANNs learn relationships between inputs and outputs by adjusting connection weights during training.

Example: An ANN may predict distillation overhead purity from feed temperature, reflux ratio, feed composition, pressure, and tray efficiency.

Basic Structure of a Neural Network

A **neural network** typically has three main types of layers:

- **Input Layer:** Where data enters the network. Each node in this layer represents a feature or variable in the input data.
- **Hidden Layers:** Layers between the input and output. They process the data using weights and activation functions. There can be one or many hidden layers depending on the task.
- **Output Layer:** Produces the final result, such as a prediction or classification.

Each connection between neurons has a weight that determines the importance of the input. As the network learns, these weights are adjusted to improve results.

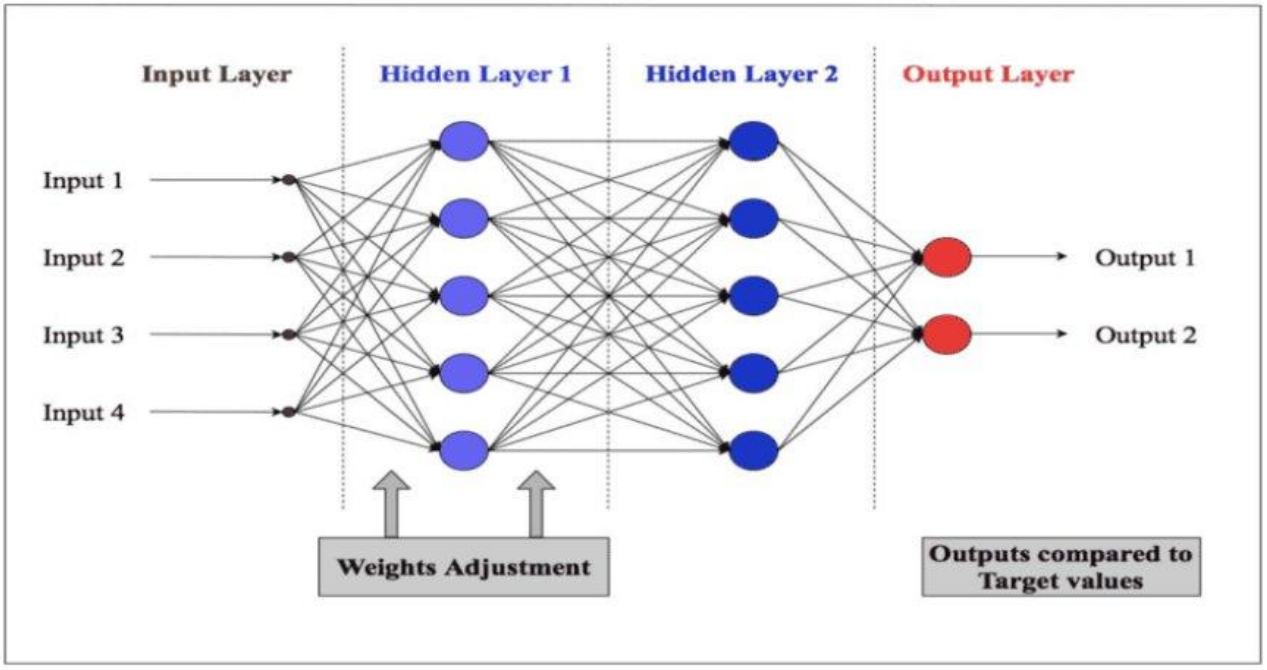


Figure 2. Typical multi-layer Artificial Neural Network (ANN) architecture showing input layers, hidden layers, output layers, interconnecting weighted pathways, and iterative weight adjustment during neural network training. (Source: Illustrative AI-assisted engineering visualization.)

Summary

Artificial Neural Networks (ANNs) enable computational systems to identify patterns, perform predictive analysis, support decision-making, and improve performance through iterative learning. These capabilities have made neural networks fundamental components of many modern Artificial Intelligence (AI) applications, including intelligent assistants, recommendation systems, predictive analytics, process optimization, and industrial automation.

Although neural networks possess certain limitations, ongoing research and technological advancements continue to improve their computational efficiency, transparency, interpretability, and practical applicability across engineering and industrial systems. A clear understanding of neural network operation provides an important foundation for exploring the broader application of AI and machine learning technologies in engineering, business, manufacturing, and digital process optimization.

Artificial Neuron: A simplified mathematical processing unit within an ANN. It receives numerical inputs, applies weights and an activation function, and produces an output.

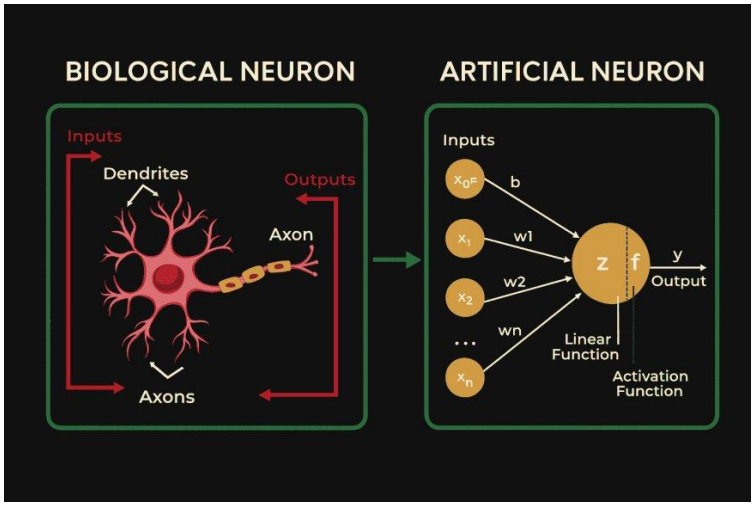


Figure 3. Comparison of biological and artificial neurons illustrating the conceptual foundation of Artificial Neural Networks (ANNs) in Artificial Intelligence and Machine Learning systems. (Source: Illustrative AI-assisted engineering visualization.)

B

Balance Equation: A mathematical expression based on conservation principles. Common engineering balance equations include mass, energy, momentum, and component balances.

Biological Intelligence: The natural ability of humans and other living organisms to perceive, learn, remember, reason, communicate, adapt, and make decisions.

How Biological Intelligence Works

Each bullet begins with a Guided Link so you can explore deeper.

- **Neural Processing** — billions of neurons communicate through electrical and chemical signals.
- **Learning & Memory** — synapses strengthen or weaken through experience (synaptic plasticity).
- **Perception** — senses convert external stimuli into neural signals.
- **Reasoning & Problem-Solving** — the brain integrates information to make decisions.

- **Emotion & Motivation** — feelings influence behaviour, learning, and judgement.
- **Adaptation** — humans adjust to new environments, challenges, and social contexts.

This intelligence is **organic**, **self-repairing**, **energy-efficient**, and shaped by **millions of years of evolution**.

Key Characteristics of Biological Intelligence

- **Embodied** — tied to a physical body and sensory system.
- **Adaptive** — learns from experience and changes behaviour.
- **Context-aware** — understands nuance, emotion, and social cues.
- **General-purpose** — can learn any skill, not just one task.
- **Self-motivated** — driven by goals, emotions, and survival instincts.
- **Conscious** — capable of awareness, intuition, and creativity.

Biological intelligence is the natural, evolved capability of living organisms — especially humans — to think, learn, adapt, and make decisions using the brain and nervous system.

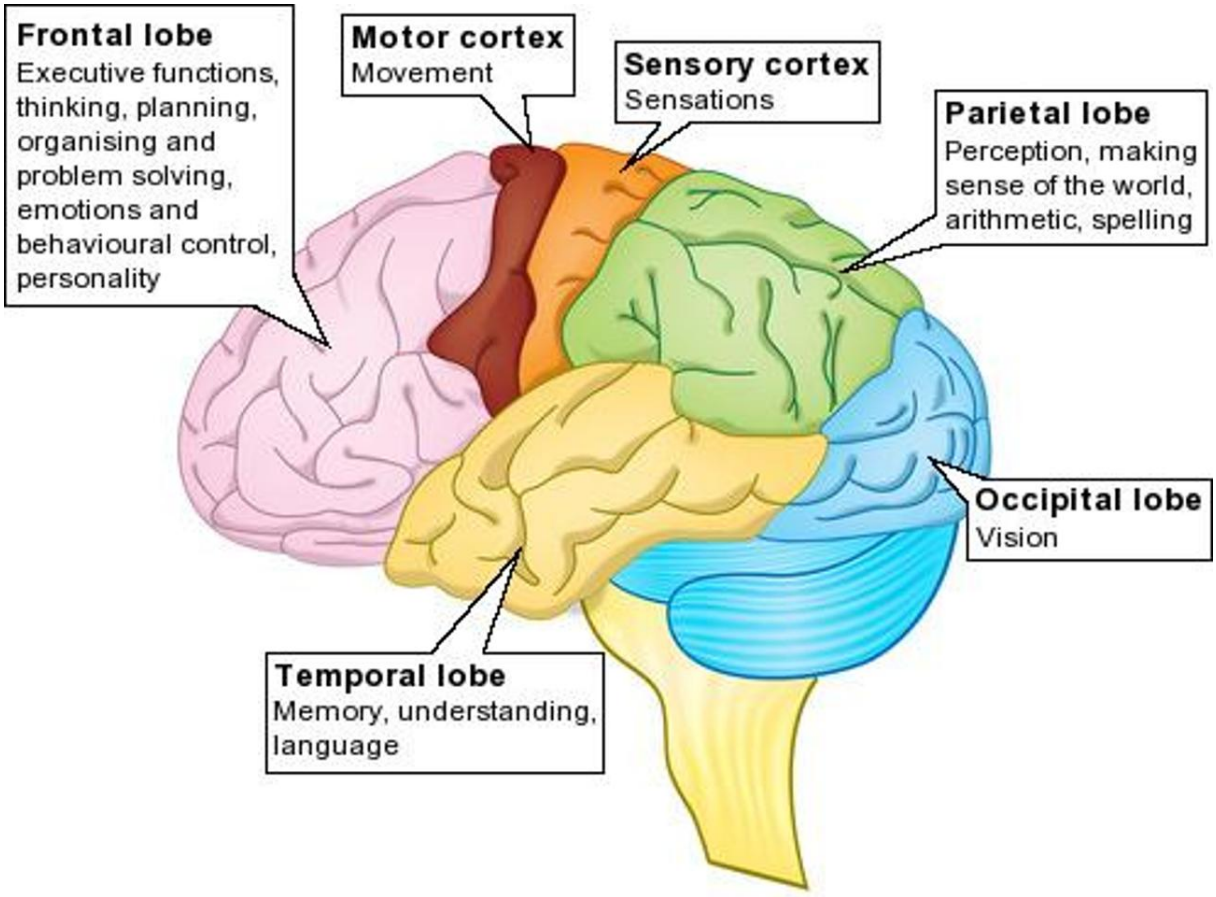


Figure 4. The four lobes of the Human Brain

Biological Neuron: A specialized living cell that receives, processes, and transmits electrical and chemical information through dendrites, the cell body, the axon, and synapses.

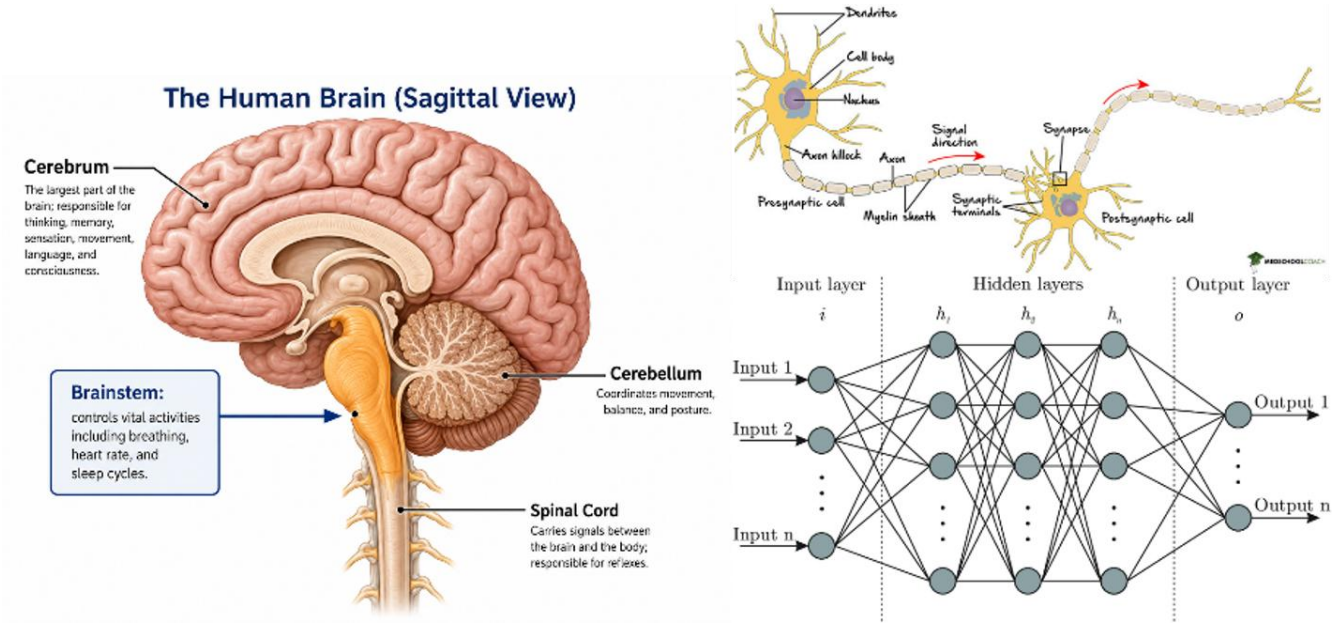


Figure 5. Composite illustration showing the human brain, a biological neuron, and an artificial neural network (ANN). The brain represents the biological foundation of intelligence; the neuron illustrates the cellular mechanism of signal transmission; and the ANN demonstrates the engineered abstraction used in modern machine-learning systems. Together, these elements highlight the conceptual bridge between natural cognition and computational learning models.

Black-Box Model: A model that can provide predictions without clearly revealing the underlying physical relationships responsible for those predictions. Many ANN and deep-learning models are described as black-box models.



Figure 6a. Black Box Process Model

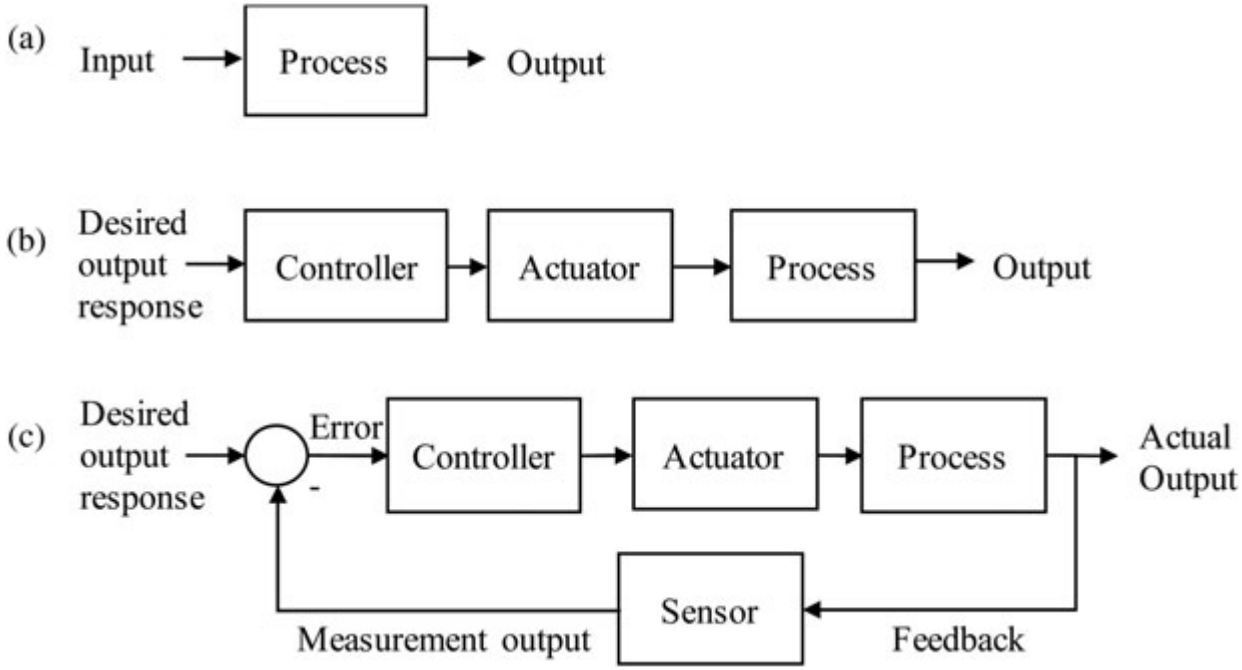


Figure 6b. Black Box Representation of System Dynamics

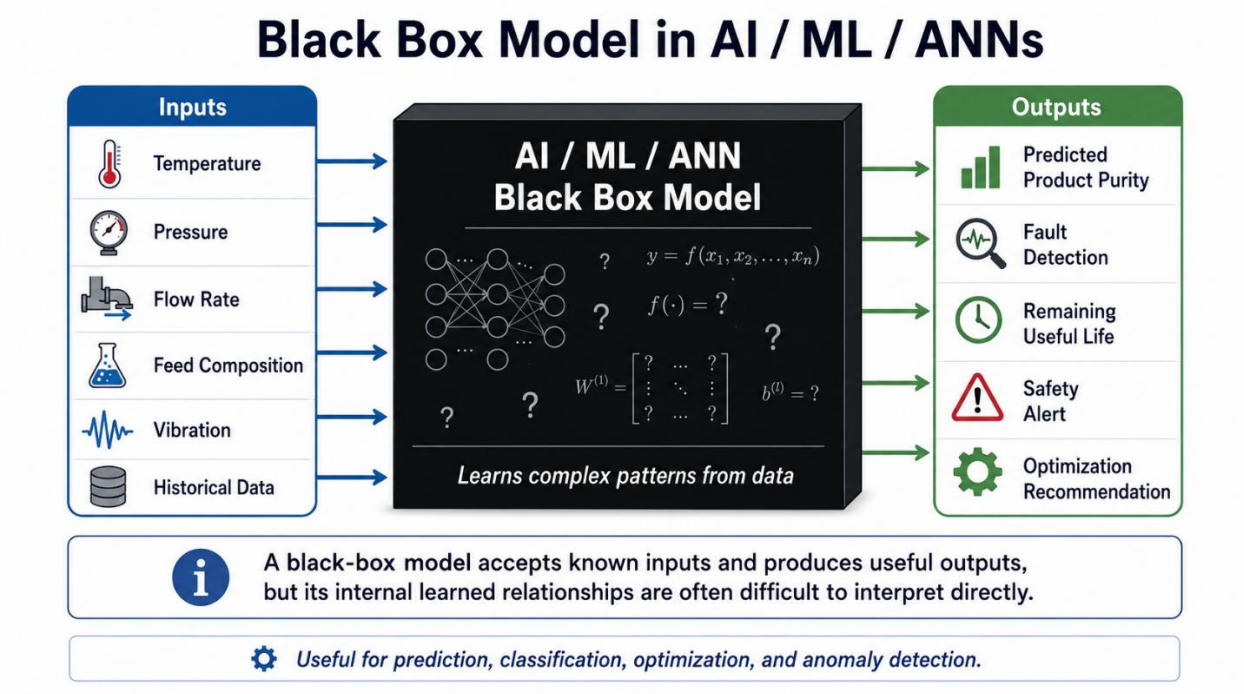


Figure 6c. Black Box Model in AI/ML/ANNs

What the image represents

- The **box** symbolizes a system whose internal structure is not examined.
- Only **input–output relationships** matter.
- Common in **process modeling**, **control systems**, **machine learning**, and **chemical engineering** when internal kinetics or mechanisms are too complex or unavailable.

Blue Hydrogen: Hydrogen produced from fossil fuels, commonly natural gas, where a substantial portion of the resulting carbon dioxide is captured, transported, utilized, or stored through CCUS.

The environmental performance of blue hydrogen depends on factors such as:

- Carbon-capture rate
- Methane leakage
- Energy required for capture and compression
- Permanence of carbon dioxide storage
- Overall lifecycle emissions

Example: A steam methane reformer fitted with carbon capture and geological storage may produce blue hydrogen.

Brainstem: The region at the base of the brain connecting the cerebrum to the spinal cord. It regulates essential automatic functions such as breathing, heart rate, blood pressure, reflexes, and sleep cycles (See Figure 6).

C

Carbon Capture: The separation of carbon dioxide from industrial gas streams before it is released to the atmosphere.

Carbon Capture, Utilization and Storage (CCUS): A group of technologies used to capture carbon dioxide from industrial processes or other emission sources, transport it, use it beneficially where appropriate, or store it permanently in suitable geological formations.

The principal stages are:

1. Carbon dioxide capture
2. Conditioning and compression
3. Transportation
4. Utilization or permanent storage

Example: Carbon dioxide produced during hydrogen manufacture may be captured, compressed, and injected into a depleted oil or gas reservoir.

Carbon Dioxide Equivalent (CO_2e): A common unit used to express the climate effect of different greenhouse gases by converting them into the equivalent amount of carbon dioxide.

Each greenhouse gas is multiplied by its Global Warming Potential over a specified time period.

Example: Methane emissions can be converted into tonnes of CO_2e to allow comparison with carbon dioxide emissions.

Carbon Footprint: The total quantity of greenhouse-gas emissions caused directly and indirectly by a person, product, activity, process, organization, or industrial facility. It is normally expressed in tonnes of carbon dioxide equivalent.

A carbon footprint may include:

- Direct fuel-combustion emissions
- Process emissions
- Purchased-electricity emissions
- Transportation emissions
- Supply-chain emissions
- Product-use and disposal emissions

Example: A refinery carbon footprint may include emissions from process heaters, boilers, hydrogen plants, flares, purchased electricity, and crude-oil transportation.

Carbon Storage: The long-term containment of captured carbon dioxide in suitable geological formations, such as depleted oil and gas reservoirs or deep saline aquifers.

Carbon Utilization: The beneficial use of captured carbon dioxide as a feedstock or process material. Possible applications include chemical manufacture, enhanced oil recovery, mineralization, and synthetic-fuel production.

Catalyst Activity: A measure of a catalyst's effectiveness in increasing the rate of a chemical reaction.

Catalyst Deactivation: The gradual loss of catalyst activity caused by mechanisms such as fouling, poisoning, sintering, or coke deposition. AI models may predict when catalyst performance will decline below an acceptable level.

Cause and Effect: **a**. is the logical relationship between an initiating event (**cause**) and the resulting outcome (**effect**). **b**. Cause and effect is the relationship between two events where one event (the cause) makes another event (the effect) happen.

In petroleum and petrochemical operations, this relationship is foundational for:

- Process safety
- Root cause analysis
- Control system design
- AI assisted troubleshooting
- HAZOP and LOPA

1. The Meaning of Cause

A cause is the initiating condition, failure, or deviation that triggers a sequence of events.

Examples in refinery/petrochemical systems:

- Pump seal failure

- Exchanger fouling
- High reactor temperature
- Loss of cooling water
- AI detected anomaly in compressor vibration

These are initiators.

2. The Meaning of “Effect”

An effect is the outcome or consequence that results from the cause.

Examples:

- Loss of containment
- Reduced heat transfer efficiency
- Reactor runaway
- Trip of a major compressor
- Increased energy consumption

- Safety instrumented system activation

These are consequences.

3. Cause and Effect in Process Safety

C&E relationships are the backbone of:

- Cause and Effect Matrices
- Safety Instrumented Functions (SIFs)
- Emergency shutdown logic (ESD)
- Fire and gas detection systems

Example:

Cause Effect

High pressure in reactor ESD valve closes, feed pump trips

Loss of cooling water Reactor temperature rises → SIS activates

Gas leak detected Isolation valves close, alarms activate

4. Cause and Effect in AI/ML Systems

AI enhances C&E analysis by:

- Detecting hidden causes (patterns humans miss)
- Predicting effects before they occur
- Ranking causes by probability
- Suggesting corrective actions

Examples:

- AI predicts exchanger fouling → effect: reduced heat recovery
- ML detects abnormal compressor vibration → effect: potential trip
- Digital twin identifies steam imbalance → effect: energy inefficiency

AI strengthens both diagnostics (finding causes) and prognostics (predicting effects).

5. Cause and Effect in Energy and Heat Integration

Heat Integration

- Cause: Exchanger fouling
- Effect: Reduced heat recovery → higher furnace duty → higher fuel use

Energy Integration

- Cause: Steam header pressure drop
- Effect: Turbine efficiency loss → increased power import → higher energy cost

6. The Importance of Cause and Effect

It enables engineers to:

- Prevent incidents
- Improve reliability
- Optimise energy use

- Strengthen AI assisted decision making

- Design safer, more resilient systems

Cause and Effect thinking is a core human centered skill that complements AI.

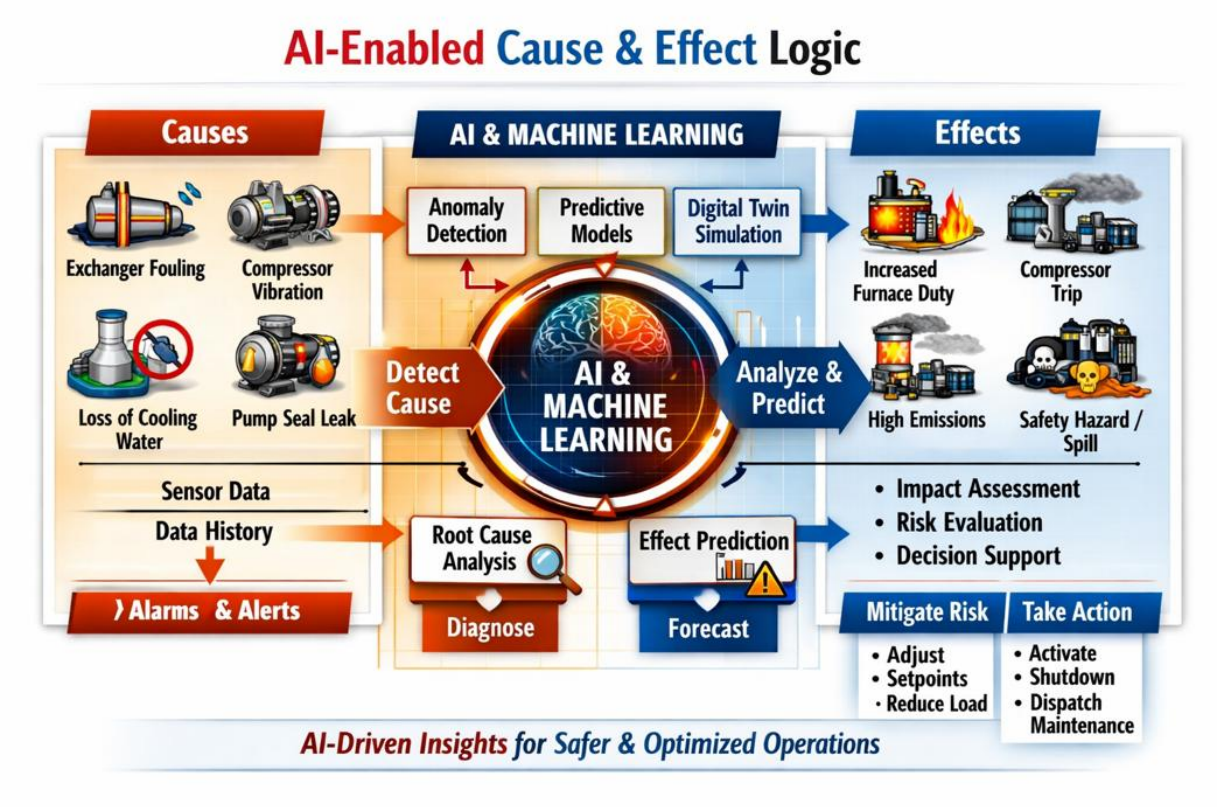


Figure 7. AI Enabled Cause and Effect Logic in Process Safety and Optimization (Source: Author's illustrative visualization developed with AI-assisted tools.)

Cell Body: The central part of a biological neuron that processes incoming signals and supports the neuron's essential functions. It is also known as the soma (Figure 6).

Cerebellum: The region at the lower rear of the brain responsible for balance, movement coordination, timing, precision, and motor learning. In an engineering analogy, it acts like a performance-optimization and coordination system.

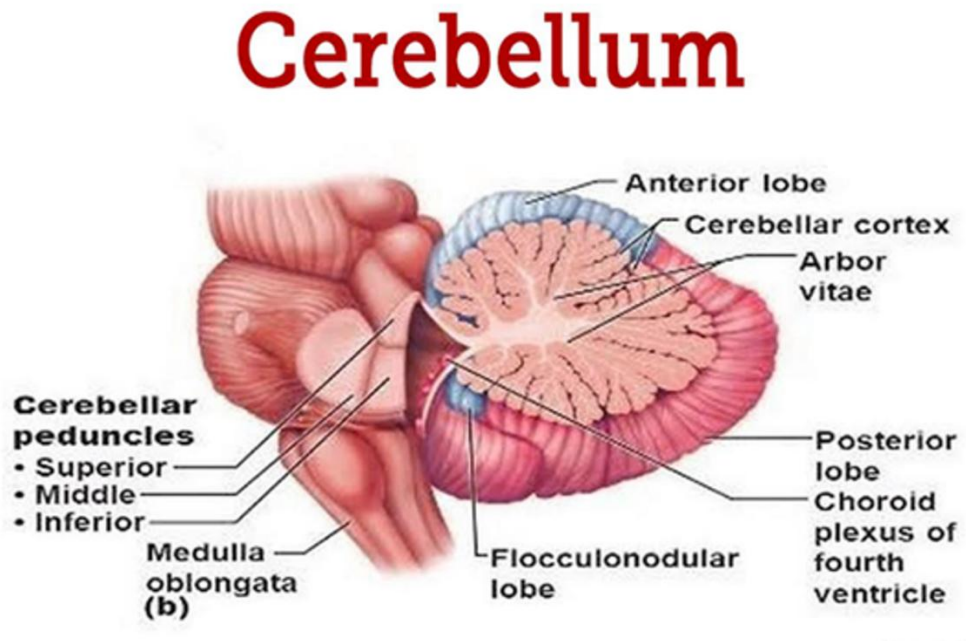


Figure 8. The Cerebellum is located at the lower rear portion of the brain, beneath the cerebrum. Although much smaller than the cerebrum, it contains

more than half of the brain's neurons. It is responsible for coordinating movement and balance, and ensures that activities are smooth and accurate.

Cerebrum: The largest part of the human brain and the principal centre for higher cognitive functions, including reasoning, memory, perception, language, creativity, planning, and decision-making.

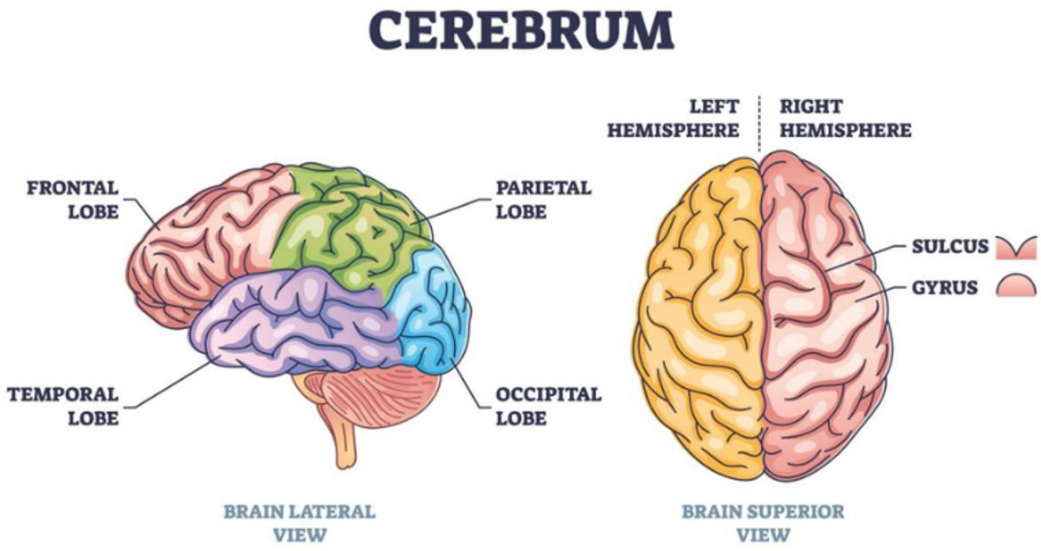


Figure 9. The Cerebrum (The Largest Part of the Brain) The Cerebrum occupies the upper and front portions of the brain and accounts for approximately 85% of the brain's mass. The Corpus Callosum connects the two hemispheres, which enables them to communicate with one another without any difficulty.

Classification: A machine-learning task in which data are assigned to predefined categories.

Example: Classifying equipment behaviour as normal, warning, alarm, or failure.

Cloud Computing: The remote provision of computing power, software, storage, and analytics through networked computer systems. Cloud platforms may support industrial data analysis and large-scale AI model training.

Cognition: The mental processes involved in acquiring knowledge, understanding information, learning, remembering, reasoning, communicating, solving problems, and making decisions.

Cognitive functions: **a**. are the mental processes that enable humans to perceive, think, learn, reason, remember, solve problems, communicate, and make decisions. They represent the brain's ability to process information and respond intelligently to situations, experiences, and challenges.

In simple terms, cognitive functions are the "thinking and understanding" activities of the human mind. **b**. Cognitive functions are the mental processes the human brain uses to perceive, interpret, remember, decide, communicate,

and learn. They form the foundation of human intelligence, enabling engineers to solve problems, make judgments, innovate, and collaborate.

These functions map naturally to AI/ML capabilities, which is why your presentation theme is so powerful.

The Five Core Cognitive Functions

Each function includes a Guided Link so you can expand it instantly.

1. Perception: The ability to sense and interpret information from the environment. In engineering: reading gauges, interpreting alarms, recognizing patterns in plant behaviour.

AI analogue: sensor fusion, computer vision.

2. Memory and Pattern Recognition: Storing, recalling, and recognizing relationships in information. In engineering: recalling past incidents, recognizing abnormal trends.

AI analogue: machine learning models.

3. Decision-Making and Planning: Evaluating options, predicting outcomes, and choosing actions. In engineering: adjusting operating conditions, troubleshooting, risk assessment.

AI analogue: decision engines, optimization algorithms.

4. Language and Communication: Understanding and expressing ideas through speech, writing, and symbols. In engineering: writing reports, giving instructions, collaborating across teams.

AI analogue: natural language processing (NLP).

5. Learning and Adaptation: Improving knowledge and skills through experience and feedback. In engineering: continuous improvement, learning from near-misses, adapting to new technologies.

AI analogue: deep learning, reinforcement learning, digital twins.

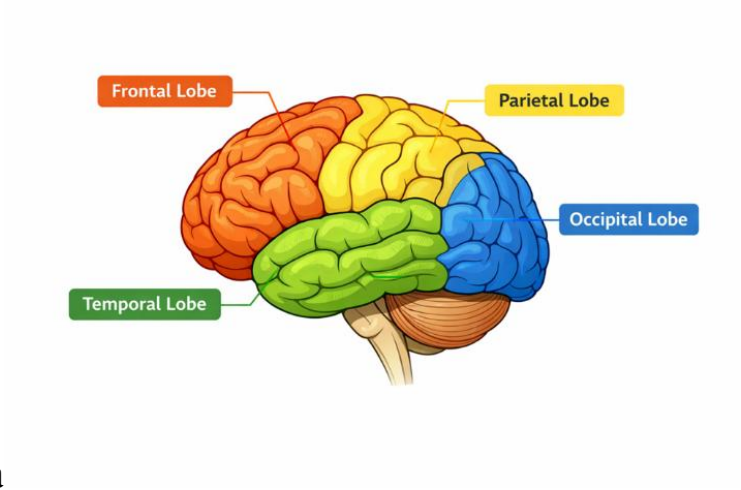
Cognitive functions and their importance in engineering.

Chemical and process engineers rely on cognitive functions every day:

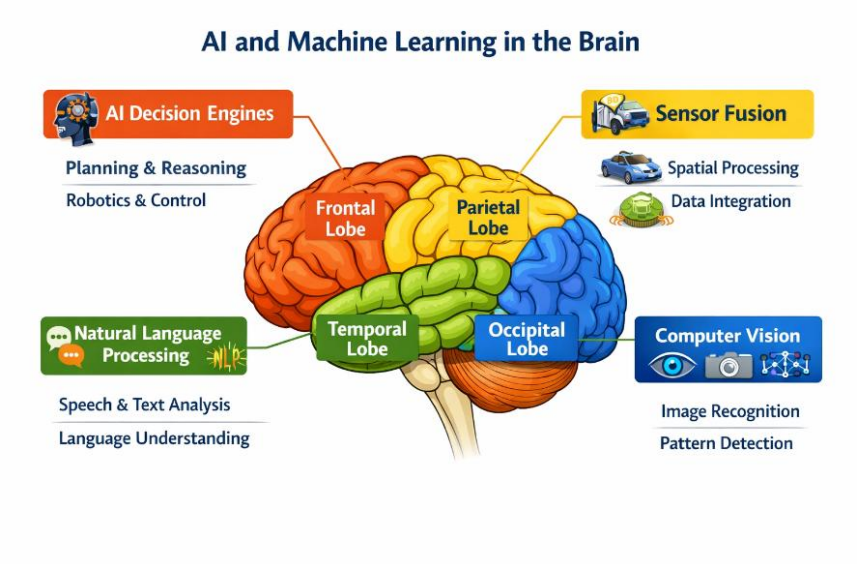
- Perception → interpreting sensor data
- Memory → recalling past plant behaviour
- Decision-making → adjusting process conditions
- Communication → coordinating with operators and management
- Learning → improving safety and efficiency

These human abilities are **amplified** when paired with AI/ML systems.

Cognitive Functions + AI/ML = Modern Engineering Practice



a



b

Figure 10. **a**. Human brain in four-lobes. **b**. Al and Machine Learning in the brain. (Source: Author's illustrative visualization developed with AI-assisted tools.)

Communication: Is the ability to **convey ideas clearly, listen actively, and create shared understanding** across teams, disciplines, and organisational levels. In today's engineering world—where AI, digital tools, and global collaboration shape daily work—communication is not just a soft skill. It is a **core engineering competency** that determines safety, efficiency, innovation, and leadership effectiveness.

1. Understanding the Essence of Communication

Communication in engineering is the disciplined practice of:

- **Clarity of expression** — making complex ideas understandable
- **Active listening** — understanding before responding
- **Audience awareness** — tailoring the message to operators, managers, or researchers
- **Feedback exchange** — giving and receiving information constructively
- **Structured thinking** — organising ideas logically

Communication is not just talking. It is **creating alignment**.

2. The Significance of Communication in Engineering

Engineering decisions affect:

- Safety
- Production
- Reliability
- Cost
- People

Strong communication ensures:

- Fewer misunderstandings
- Better shift handovers
- Clearer operating instructions
- Faster problem-solving
- Stronger collaboration
- Better adoption of AI tools

Communication is the **bridge** between technical knowledge and operational execution.

3. Communication in the Age of AI

AI changes how information flows, but communication remains human-led.

AI can:

- Summarise data
- Generate reports
- Analyse patterns
- Provide recommendations

But AI cannot:

- Build trust
- Sense team dynamics
- Understand emotional nuance
- Replace human judgment
- Inspire action

This is why engineers must combine:

- AI literacy
- Human-centered communication
- Emotional intelligence

- Ethical judgment

AI improves communication; humans provide its significance.

4. Communication in Refinery and CPI Operations

Communication is the backbone of:

- Shift handovers
- Permit-to-work systems
- Incident reporting
- Maintenance coordination
- Start-up and shutdown procedures
- Safety meetings and toolbox talks
- AI-assisted operational decisions

Examples:

- An operator explaining an abnormal trend to an engineer
- A process engineer presenting AI-generated insights to management
- A maintenance team coordinating a critical repair
- A cross-functional team evaluating an AI recommendation

Clear communication prevents accidents and improves performance.

5. Core Communication Skills for Engineers

Each item includes a Guided Link for deeper exploration.

- **Technical writing** — clear procedures, reports, and documentation
- **Presentation skills** — conveying ideas with confidence
- **Concise messaging** — saying more with fewer words
- **Constructive dialogue** — resolving disagreements productively
- **Cross-disciplinary communication** — bridging engineering, operations, and management
- **Non-verbal communication** — tone, posture, presence

These skills elevate engineers from technical contributors to **influential communicators**.

6. Summary

Communication is the **lifeblood** of engineering practice.

It ensures that:

- AI insights are understood and trusted

- Teams operate safely and efficiently
- Leaders inspire and guide
- Innovation spreads
- People feel heard and valued

In a world where AI accelerates information, communication accelerates **understanding**.

Computer Vision: An AI capability that enables computers to interpret images or video.

Example: Detecting corrosion, leaks, flames, damaged insulation, or unsafe worker behaviour from camera images.

Condition Monitoring: The continuous or periodic assessment of equipment condition using measurements such as vibration, temperature, pressure, flow, acoustic signals, and lubricant properties.

Continuous Stirred Tank Reactor (CSTR): A reactor in which feed enters continuously, products leave continuously, and the contents are assumed to be well mixed.

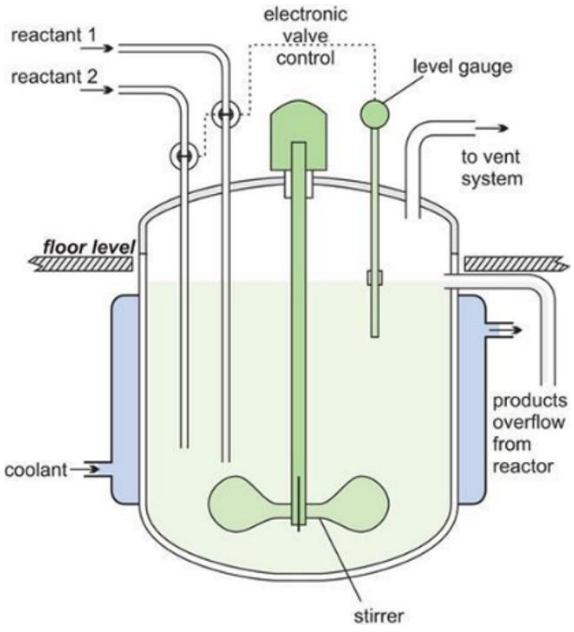


Figure 11. A continuous stirred tank reactor (CSTR)

Convolutional Neural Network (CNN): A deep-learning architecture particularly suited to images, thermal scans, spatial data, and spectrograms.

Example: A CNN may analyse thermal images to identify hot spots or corrosion damage.

Corpus Callosum: The structure that connects the left and right hemispheres of the cerebrum, allowing communication between them (Figure 11).

Creativity: The ability to generate original ideas, develop new approaches, and improve existing designs or systems. Generative AI can assist creativity, but human judgment determines whether the proposed idea is useful and safe.

Creative Thinking: is the ability to generate new ideas, reframe problems, and imagine possibilities beyond conventional boundaries. In today's AI-driven, digitally transformed world facing complex global issues, creativity is essential. It is a **strategic capability** that drives innovation, resilience, and competitive advantage.

1. Understanding Creative Thinking

Creative thinking is the disciplined ability to:

- **See problems differently** — shifting perspective to reveal new solutions
- **Generate novel ideas** — producing multiple, diverse possibilities
- **Connect unrelated concepts** — combining ideas in unexpected ways
- **Challenge assumptions** — questioning “the way we’ve always done it”
- **Imagine alternatives** — exploring what could be, not just what is

Creative thought is separate from artistic talent. **It reflects a person’s ability to think flexibly and adapt ideas in new ways.**

2. The Importance of Creative Thinking in Engineering

Engineering is fundamentally a problem-solving discipline. Creative thinking enables engineers to:

- Design better processes
- Improve safety and reliability
- Reduce energy consumption
- Innovate new technologies
- Solve complex, ambiguous problems
- Adapt to rapidly changing environments

Creative thinking ignites the innovations that transform engineering practice.

3. Creative Thinking in the Age of AI

AI expands the creative capacity of engineers by:

- Generating design alternatives
- Simulating scenarios
- Identifying hidden patterns
- Suggesting optimisations
- Accelerating experimentation

But AI cannot:

- Define the problem
- Imagine the future

- Understand human needs
- Make value-based decisions
- Replace human intuition

This is why modern engineers must combine classical engineering judgment with emerging digital tools:

- AI-assisted creativity
- Human imagination
- Ethical judgment
- Emotional intelligence

AI enhances creativity, yet **human judgment guides the outcome**.

4. Creative Thinking in Refinery and CPI Operations

Creative thinking drives innovation in:

- Heat-exchanger optimisation
- Energy efficiency improvements
- Fouling mitigation strategies
- Digital twin development
- AI-assisted process control

- Turnaround planning
- Safety system redesign

Examples:

- Reimagining a fouling-cleaning strategy using AI and Python
- Designing a new workflow for shift handovers
- Creating a predictive maintenance model for rotating equipment
- Developing a novel catalyst monitoring method

Creative thinking transforms constraints into **opportunities**.

5. Core Creative Thinking Skills for Engineers

Each item outlines an essential component of effective creative thinking.

- **Brainstorming** — generating many ideas quickly
- **Divergent thinking** — exploring multiple directions
- **Convergent thinking** — selecting the best ideas
- **Design thinking** — human-centred problem solving
- **Systems creativity** — innovating across interconnected systems
- **Scenario imagination** — envisioning future possibilities

These skills help engineers innovate with purpose and precision.

Critical Thinking: **a.** is the disciplined ability to **analyse information, question assumptions, evaluate evidence, and make sound, defensible decisions**. **b**. the skill of evaluating information objectively to reach clear, rational conclusions. **c**. the process of breaking down complex problems to determine the most reliable and defensible solution. **d**. is the ability to effectively analyze information and form a judgment. **e**. is the ability to analyse information objectively, question assumptions, and evaluate evidence before forming a conclusion.

Instead of accepting ideas at face value, it involves examining facts and arguments, identifying biases, and considering multiple perspectives to understand a situation.

In today's engineering world where AI accelerates data, complexity increases, and consequences are high, critical thinking is the systematic examination of complex issues to reach the soundest conclusion.

The following are aspects of Critical Thinking:

1. Understanding Critical Thinking in Engineering Decision-Making

Critical thinking is the structured process of:

- **Questioning assumptions** — not accepting information at face value
- **Evaluating evidence** — distinguishing facts from opinions
- **Analysing systems** — understanding interactions and consequences
- **Reasoning logically** — drawing conclusions based on sound principles
- **Making informed judgments** — choosing the best path under uncertainty

Critical thinking is not about being sceptical; it is about being **rigorous, curious, and precise**.

2. The Importance of Critical Thinking in Engineering

Engineering decisions affect:

- Safety
- Reliability
- Cost
- Environment
- People

Critical thinking ensures engineers can:

- Interpret complex data
- Challenge flawed assumptions
- Identify root causes
- Evaluate AI recommendations
- Make decisions under pressure
- Avoid cognitive biases

It is the **cognitive framework** that supports engineering judgment**.**

3. Critical Thinking in the Age of AI

AI provides information. Critical thinking provides **interpretation**.

AI can:

- Analyse large datasets
- Predict failures
- Optimise operations
- Generate recommendations

But AI cannot:

- Understand context
- Weigh ethical implications

- Judge trade-offs
- Detect organisational pressures
- Replace human reasoning

This is why engineers must combine:

- AI literacy
- Human-centred reasoning
- Ethical judgment
- Emotional intelligence

AI accelerates thinking, but **critical thinking ensures it is correct**.

4. Critical Thinking in Refinery and CPI Operations

Critical thinking is essential for:

- Process safety decisions
- Troubleshooting abnormal operations
- Evaluating AI-generated insights
- Root-cause analysis (RCA)
- Turnaround planning
- Risk assessments (HAZOP, LOPA)

- Incident investigations

Examples:

- An AI model recommends reducing furnace duty—should the operator follow it?
- A heat exchanger shows declining performance—is it fouling, instrumentation error, or crude variability?
- A near-miss occurs—what systemic factors contributed?

Critical thinking ensures decisions are **accurate, safe, and defensible**.

5. Core Critical Thinking Skills for Engineers

Each item outlines an essential component of effective critical thinking.

- **Analytical reasoning** — breaking problems into components
- **Root-cause thinking** — identifying underlying issues
- **Evidence-based decision-making** — relying on data, not assumptions
- **Bias awareness** — avoiding mental shortcuts
- **Scenario evaluation** — comparing multiple possible outcomes
- **Systems thinking** — seeing the whole, not just the parts

These skills elevate engineers from problem-solvers to **strategic thinkers**.

6. Conclusion

Critical thinking is the **structured discipline** that ensures engineering decisions are:

- Safe
- Ethical
- Evidence-based
- Context-aware
- Technically sound

In a world where AI accelerates information, critical thinking accelerates **wisdom**.

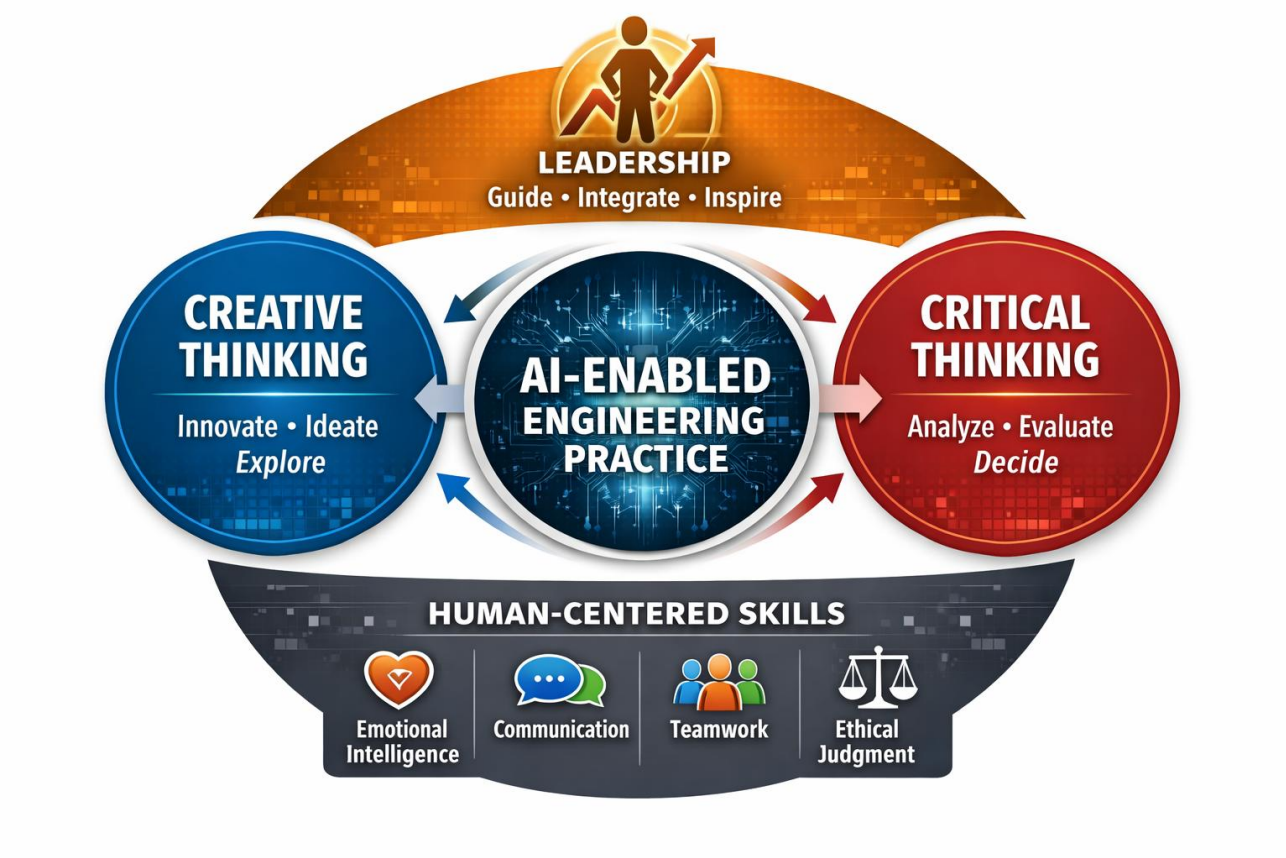


Figure 12. Integrating Creative and Critical Thinking with AI-Driven Leadership and Human-Centered Skills (Source: Author's illustrative visualization developed with AI-assisted tools.)

Crude Assay: A detailed laboratory characterization of a crude oil used to determine its physical properties, chemical composition, boiling-range distribution, contaminants, and expected refinery-product yields.

A crude assay may contain information on:

- API gravity
- Sulfur content

- Nitrogen content
- Metals content
- Salt content
- Viscosity
- Pour point
- Carbon residue
- True boiling-point distribution
- Product yields
- Properties of individual boiling fractions

Example: A refinery uses crude-assay data to estimate the quantities and properties of naphtha, kerosene, diesel, gas oil, and residue that may be obtained from a crude oil.

Crude Distillation Unit (CDU): The principal refinery unit that separates crude oil into fractions according to boiling range. It is the primary refinery system where **raw crude oil is heated and separated** into various petroleum fractions. The process begins by preheating the crude oil through a series of heat exchangers, then sending it to a **distillation column** operating at **atmospheric pressure**. Inside the column, the crude oil vaporizes and rises through trays or packing, separating into products according to their boiling ranges.

A CDU is the front-end separation system of a petroleum refinery, responsible for breaking down raw crude oil into fundamental hydrocarbon fractions based on their boiling ranges. The process begins with desalting to remove salts and water, followed by progressive heating through a preheat train that recovers energy from product streams. The crude is then routed to the furnace, where it is heated to approximately 340–370°C to vaporize lighter components without inducing thermal cracking. This vapor–liquid mixture enters the atmospheric distillation column, a tall fractionation tower equipped with trays or packing that enables separation through controlled vapor–liquid contact. Overhead systems condense the lightest vapors into wet gas, naphtha, and reflux, while intermediate fractions such as kerosene, diesel, and atmospheric gas oil are withdrawn through side draws and stabilized in side strippers.

The heaviest material, atmospheric residue, collects at the bottom of the column and is routed to the Vacuum Distillation Unit (VDU) for further separation into vacuum gas oils and vacuum residue. Throughout the CDU, pumparounds and heat-recovery exchangers enhance energy efficiency by transferring heat from product streams back into the crude feed. The CDU establishes the refinery's overall product slate and supplies essential feedstocks to downstream units such as hydrotreaters, catalytic reformers, fluid catalytic crackers (FCC), and hydrocrackers. As the refinery's primary separation step, the CDU plays a

critical role in determining operational flexibility, product yields, and overall refinery performance.

Key outputs typically include:

- **Light gases** (fuel gas)
- **Naphtha** (gasoline blending component)
- **Kerosene** (jet fuel)
- **Diesel**
- **Atmospheric gas oil**
- **Residue** (sent to vacuum distillation or conversion units)

Why the CDU is important:

- It defines the **initial breakdown** of crude oil into usable streams.
- It feeds downstream units like **hydrotreaters**, **reformers**, **FCC**, **hydrocrackers**, and **vacuum distillation units**.
- It sets the **overall refinery yield structure**.

Table 6. Typical Product Streams from a CDU

Fraction	Boiling Range (°C)	Use
Fuel Gas	< 30	Refinery fuel
Light Naphtha	30–90	Gasoline blending
Heavy Naphtha	90–180	Reforming feed
Kerosene	180–240	Jet fuel
Diesel	240–360	Diesel fuel
Atmospheric Gas Oil	360–400	FCC feed
Atmospheric Residue	> 400	VDU feed

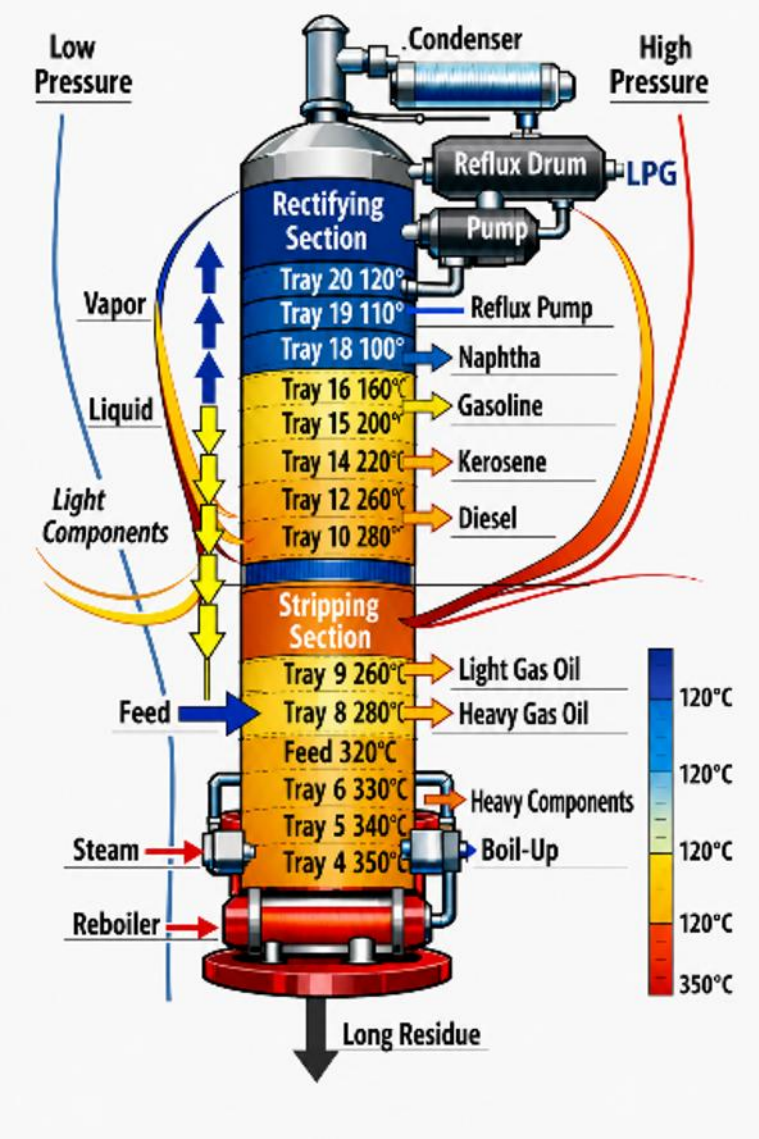


Figure 13. A Crude distillation unit showing equipment items, light components, heavy components, temperature and pressure profiles, and products.

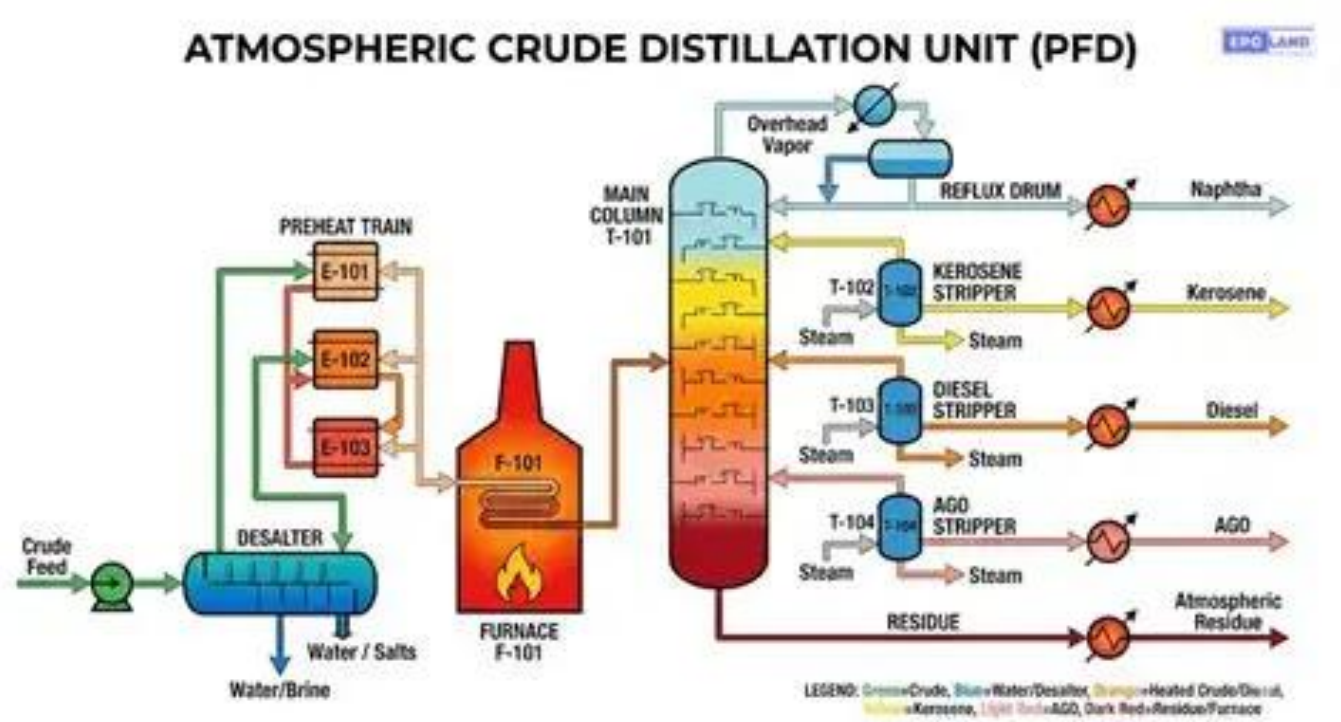


Figure 13b. CDU Process Flow Diagram

D

Data Analyst: A Data Analyst is a professional who collects, processes, and interprets data to help organizations make informed decisions. They transform raw data into actionable insights using statistical methods, visualization tools, and computational techniques. Data analytics plays a vital role in modern process industries, where engineers handle vast amounts of operational data.

Data analysts form the **bridge between raw data and intelligent systems**. In chemical/process engineering:

- **AI** automates data interpretation and decision-making.
- **ML** learns from historical process data to predict future outcomes.
- **Data analysts** ensure the data feeding these models is accurate, relevant, and meaningful.

Together, they enable **data-driven engineering**, where decisions are guided by continuous learning and optimization.

Data Analytics: Is the **systematic examination of data** to extract meaningful insights, identify patterns, and support decision-making.
In engineering, it involves **collecting, cleaning, and interpreting process data** from sensors, control systems, and laboratory analyses to improve plant performance and safety.

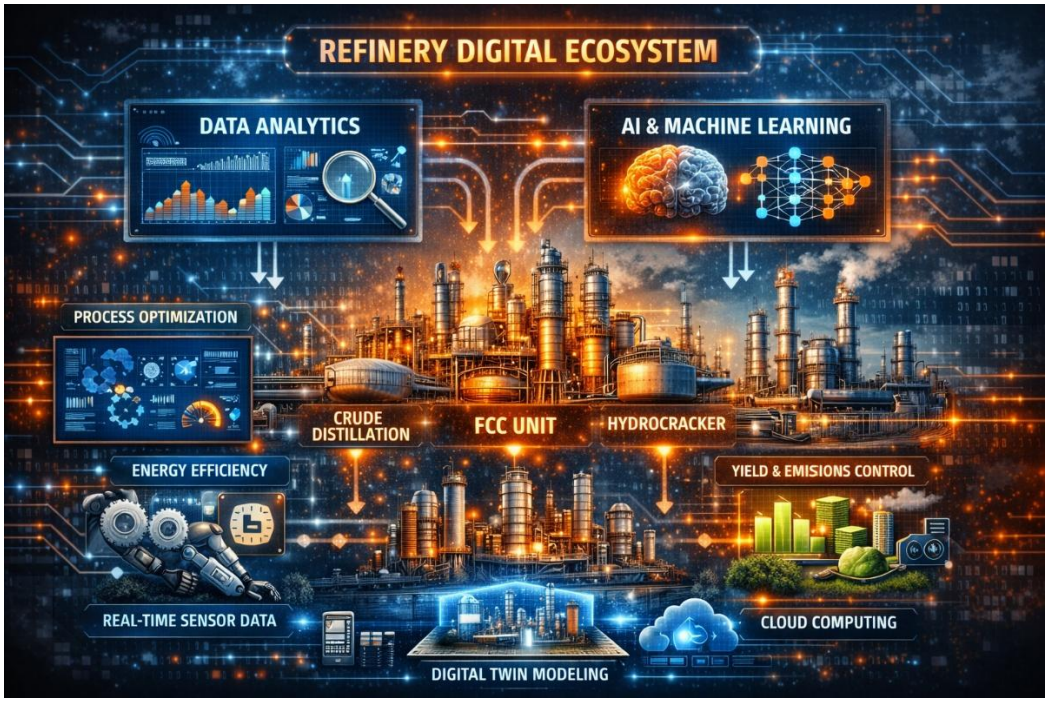


Figure 14. Refinery Digital Eco-system with Data Analytics, AI, ML and Process Units (Source: Author's illustrative visualization developed with AI-assisted tools.)

Importance in Chemical Engineering

Data Analytics is now a **core competency** for modern chemical engineers. It bridges traditional process design with digital intelligence by enabling:

- **Process Optimization:** identifying inefficiencies and improving yield, energy use, and throughput.
- **Predictive Maintenance:** forecasting equipment failures using vibration, temperature, and pressure data.

- **Safety and Risk Analysis:** detecting abnormal trends and preventing incidents.
- **Quality Control:** ensuring product consistency through statistical monitoring.
- **Environmental Compliance**: tracking emissions and waste streams to meet sustainability targets.

Data Augmentation: The generation or modification of training data to increase the size or diversity of a dataset.

Example: A GAN may generate representative examples of rare cooling failures when actual plant-failure data are limited.

Data-Driven Model: A model that learns relationships from historical, laboratory, simulated, or real-time data rather than relying entirely on first-principles equations.

Data Processing: **a.** Is the systematic transformation of raw industrial data into meaningful engineering information. **b**. is the systematic collection, cleaning, transformation, and organization of raw data into a usable form that supports analysis, modelling, and decision-making. It is the **foundation** of all AI/ML workflows because models can only learn from **clean, structured, meaningful data**.

Core Stages of Data Processing

- **Data Collection** — acquiring data from sensors, logs, instruments, and databases
- **Data Cleaning** — removing noise, errors, missing values
- **Data Transformation** — scaling, normalization, feature extraction
- **Data Integration** — combining data from multiple sources
- **Data Storage** — organizing data for retrieval and modelling
- **Data Preparation** — formatting data for AI/ML algorithms

Data processing is the **bridge** between raw plant data and intelligent engineering insights.

Examples for Chemical/Process Engineers

Chemical and process plants generate **massive volumes of data** from DCS/SCADA systems, analyzers, sensors, and operator logs. Data processing enables engineers to convert this raw information into actionable intelligence.

A. Process Monitoring

- Collecting temperature, pressure, flow, and composition data
- Cleaning noisy sensor readings

- Normalizing data for trend analysis
- **AI/ML link:** Clean data feeds **predictive models** for early anomaly detection

B. Predictive Maintenance

- Processing vibration, acoustic, and thermal data from rotating equipment
- Extracting features such as RMS, kurtosis, harmonics
- **AI/ML link:** Processed data trains **failure-prediction models**

C. Safety and Incident Analysis

- Cleaning and structuring alarm logs
- Converting operator narratives into analysable text
- **AI/ML link:** NLP models identify recurring hazards and root-cause patterns

D. Quality Control

- Processing lab and online analyzer data
- Removing outliers and aligning timestamps

- **AI/ML link:** ML models classify quality deviations and predict off-spec events

E. Digital Twins

- Integrating historical and real-time data
- Synchronizing time-series from multiple units
- **AI/ML link:** Deep learning models use processed data to simulate plant behaviour

Decision-Making: The cognitive process of selecting an appropriate action from several alternatives. AI may support decisions, but engineers remain responsible for the final selection.

Decision Support: The use of data, models, predictions, and recommendations to help engineers or operators make better-informed decisions.

Deep Learning: **a.** Deep Learning is a branch of machine learning (ML) that uses multi-layered artificial neural networks to learn patterns, relationships, and representations directly from large amounts of data. **b**. Is a subset of machine learning (ML) that uses neural networks with multiple layers to learn complex patterns in data. Unlike traditional machine learning, which often relies on

handcrafted features, deep learning can automatically extract features from raw data.

Unlike traditional algorithms that require manual feature selection, deep learning models **automatically extract features**, making them powerful for complex tasks such as:

- Image recognition
- Speech recognition
- Natural language processing (NLP)
- Predictive modelling
- Pattern detection in noisy or high-dimensional data

Step 1: Build Your Foundation

Deep learning builds on several core skills as:

Mathematics Basics

Mathematics is crucial for understanding how deep learning algorithms work. Focus on:

- **Linear Algebra:** Matrices, vectors, and operations. Understanding matrix multiplication is essential for neural networks.

- **Calculus:** Derivatives and gradients help in understanding optimization and backpropagation.
- **Probability and Statistics:** Concepts like probability distributions, mean, variance, and Bayes' theorem are widely used in machine learning models.

Programming Skills

Python is the most widely used language in deep learning because of its simplicity and the availability of powerful libraries like NumPy, Pandas, and Matplotlib. Learn to handle data, perform calculations, and visualize results.

Machine Learning Basics

Deep learning is a subset of machine learning, so it's important to understand basic machine learning concepts first:

- **Supervised learning:** Learning from labeled data, e.g., predicting house prices.
- **Unsupervised learning:** Finding patterns in unlabeled data, e.g., customer segmentation.
- **Key algorithms:** Linear regression, logistic regression, decision trees, and clustering algorithms.

- **Evaluation metrics:** Accuracy, precision, recall, and F1-score.

Step 2: Learn Core Deep Learning Concepts

After the foundation, the next step is to understand the core concepts of deep learning.

Neural Networks: are the building blocks of deep learning. They consist of layers of interconnected neurons that process data. Start with:

- **Perceptron:** The simplest type of neural network.
- **Feedforward Networks:** Information moves in one direction from input to output.
- **Activation Functions:** Functions like ReLU, Sigmoid, and Tanh determine how signals pass through the network.

a

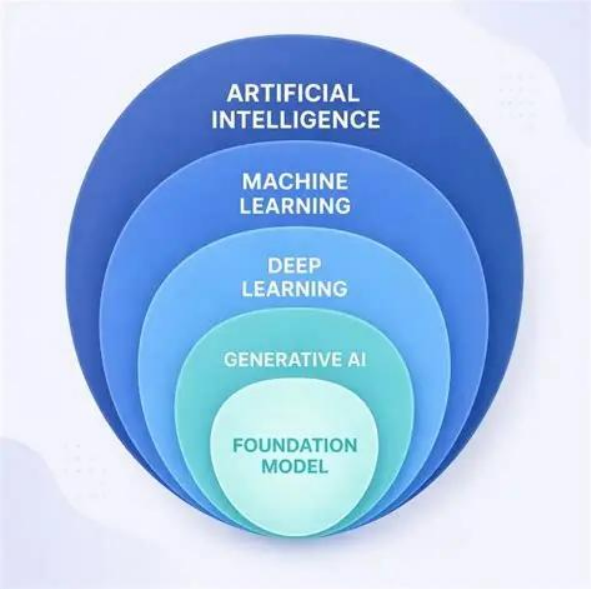


Figure 15a. Foundation Model as subset of Generative AI.

b

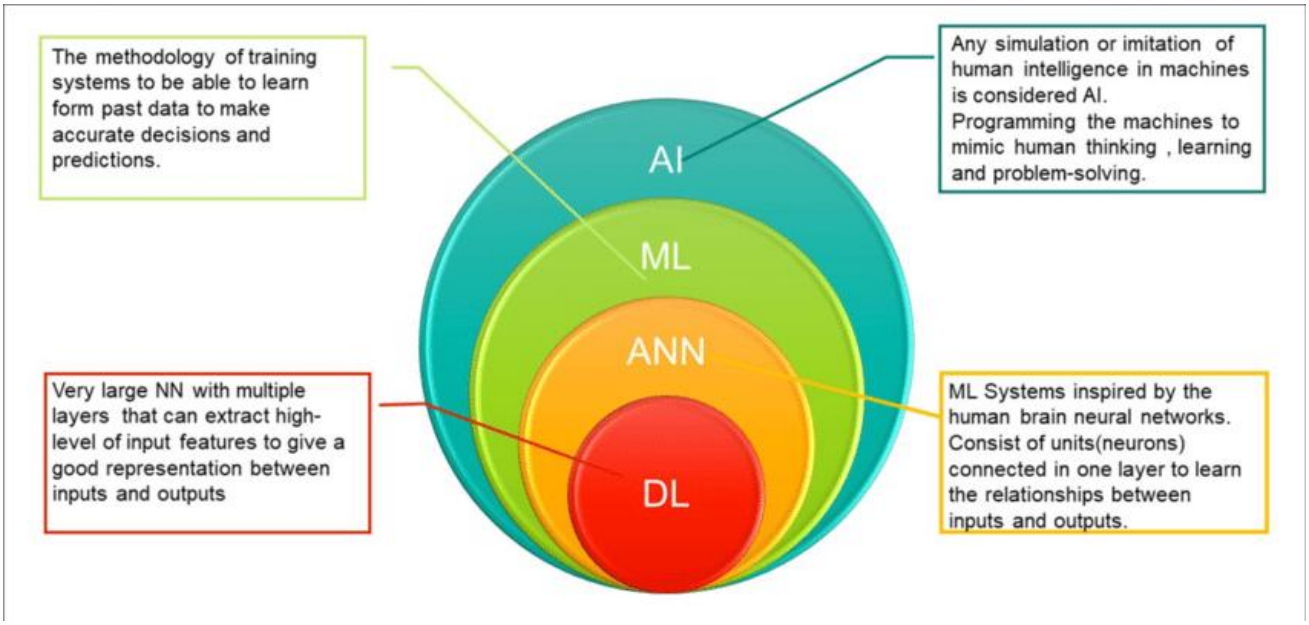


Figure 15b. Deep Learning, Artificial Neural Network, Machine Learning and Artificial Intelligence

Generative AI within the AI hierarchy

The modern AI stack is typically structured like nested boxes:

- **Artificial Intelligence (AI)** Broadest category — any system that mimics human intelligence.
- **Machine Learning (ML)** Subset of AI — systems that learn patterns from data.
- **Deep Learning (DL)** Subset of ML — neural networks with many layers.
- **Generative AI (GenAI)** Subset of DL — models that *create* new content (text, images, audio, code, etc.) based on learned patterns.

Why Generative AI is considered a Deep Learning subset

Generative AI relies on **deep neural networks**, especially:

- **Transformers** (e.g., GPT-type models)
- **Diffusion models** (e.g., Stable Diffusion)
- **GANs** (Generative Adversarial Networks)
- **VAEs** (Variational Autoencoders)

All of these are **deep learning architectures**, meaning they use multi-layer neural networks trained on massive datasets.

So generative AI is not just "part of deep learning" — it is one of the most advanced *applications* of deep learning.

Training Neural Networks

Training involves teaching the network to make accurate predictions. Key concepts include:

- **Backpropagation:** The process of adjusting weights based on errors.
- **Optimization algorithms:** Stochastic Gradient Descent (SGD), Adam, and RMSProp help improve accuracy.
- **Loss functions:** Mean Squared Error (MSE) for regression and Cross-Entropy for classification.

Regularization Techniques

Regularization helps prevent overfitting:

- **Dropout:** Randomly ignores some neurons during training.
- **Batch Normalization:** Helps stabilize and speed up training.

- **L1/L2 Regularization:** Adds penalties for large weights to encourage simpler models.

Hyperparameter Tuning

Adjusting parameters like learning rate, number of layers, and batch size can greatly affect performance. Experimenting with these settings is a crucial skill in deep learning.

Step 3: Explore Deep Learning Architectures

Different architectures are suitable for different tasks. Here's a breakdown:

Convolutional Neural Networks (CNNs)

CNNs are mainly used for image-related tasks such as classification and object detection. Key components include:

- **Convolutional layers:** Extract features from images.
- **Pooling layers:** Reduce dimensionality while keeping important information.
- **Fully connected layers:** Make the final predictions.

Recurrent Neural Networks (RNNs)

RNNs are designed for sequence data, such as text or time series. They maintain information from previous steps to influence predictions. Variants include:

- LSTM (Long Short-Term Memory)
- GRU (Gated Recurrent Unit)

These networks are widely used in natural language processing tasks like sentiment analysis or language translation.

Deep learning is increasingly used in process industries because plants generate **massive, continuous data streams** from sensors, control systems, and historical logs.

Here are engineering-specific examples:

A. Process Optimization

Deep learning models learn nonlinear relationships between variables such as temperature, pressure, flow, and composition.

- **Use case:** A **deep neural network** predicts optimal reactor conditions to maximize yield while minimizing energy consumption.

B. Predictive Maintenance

Deep learning models detect subtle patterns in vibration, acoustic, or thermal data.

- **Use case: Recurrent neural networks** forecast pump or compressor failures days or weeks before they occur.

C. Fault Detection and Anomaly Recognition

Plants often experience complex, multivariate disturbances.

- **Use case: Autoencoders** identify abnormal operating states in distillation columns or heat exchangers.

D. Soft Sensor Development

When physical sensors are expensive or impractical, deep learning can estimate unmeasured variables.

- **Use case:** A **convolutional neural network** predicts product purity or catalyst activity from indirect measurements.

E. Safety and Incident Analysis

Deep learning can interpret unstructured text and images.

- **Use case: NLP models** analyze operator logs, safety reports, and near-miss narratives to identify recurring hazards.

F. Digital Twins

Deep learning powers high-fidelity models that simulate plant behaviour.

- **Use case:** A **hybrid deep learning model** predicts dynamic responses of reactors or separation units for training and optimization.

Dendrites: Branch-like structures of a biological neuron that receive signals from other neurons. In the ANN analogy, dendrites represent input channels. (see Figures 18f, 22)

Deterministic Model: A model in which the same inputs and assumptions produce the same outputs. Deterministic process simulators rely on first-principles equations.

Digitalization: Digitalization refers to the integration of digital technologies into industrial operations, engineering workflows, manufacturing systems, and decision-making processes. It involves transforming traditional engineering operations into data-driven and digitally connected systems.

Digitalization includes:

- smart sensors,

- cloud computing,
- Industrial Internet of Things (IIoT),
- digital twins,
- AI systems,
- advanced automation,
- robotics,
- real-time monitoring systems, and
- integrated plant information systems.

Digital Twin: a. is a **virtual, real-time digital replica** of a physical asset, process, or entire facility. The key idea is that the digital model continuously mirrors what is happening in the real world using live data from sensors, IoT devices, and control systems. **b.** is a living, breathing digital copy of a machine, plant, or process that updates itself automatically as the real system changes. **c**. is a **virtual version of a real product, process, or system**, updated continuously with real-world data so engineers can monitor, simulate, and optimize performance.

Digital Twin Applications in Chemical Engineering

For chemical engineers, digital twins are used to:

- Model **distillation columns**, reactors, heat exchangers
- Predict fouling, corrosion, and equipment degradation
- Optimize energy use and process efficiency
- Simulate plant upsets and emergency scenarios
- Train operators in a safe virtual environment

Distributed control systems (DCS): A Distributed Control System (DCS) is an industrial automation architecture in which control functions are distributed across multiple interconnected controllers rather than centralized in a single unit. It provides real-time monitoring, control, data acquisition, and coordination of complex chemical and process operations.

1. Core Definition

A **Distributed Control System** is a network of controllers, sensors, actuators, and operator interfaces that work together to:

- Monitor process variables
- Execute control strategies
- Maintain safe and stable operations
- Provide operators with real-time visibility

- Coordinate multivariable interactions across the plant

Unlike a single-loop controller, a DCS spreads intelligence across the plant, improving **reliability, scalability, and fault tolerance**.

2. Key Components of a DCS

Each item represents a key dimension of DCS.

- **Field Devices** — sensors, transmitters, valves
- **Local Controllers** — distributed control modules executing PID/APC logic
- **Human–Machine Interface (HMI)** — operator consoles and graphics
- **Engineering Workstations** — configuration, tuning, diagnostics
- **Communication Network** — high-speed, redundant data links
- **Historian** — long-term storage of process data

3. DCS in Chemical/Process Engineering

DCS is the plantwide platform that integrates monitoring and control. Examples include:

A. Distillation Columns

- Controls reflux, reboiler duty, tray temperatures
- Manages interactions between pressure, composition, and flow
- Ensures stable separation and product quality

B. Reactors

- Maintains temperature, feed ratios, catalyst activity
- Handles exothermic behaviour and safety interlocks

C. Heat Exchangers and Furnaces

- Controls outlet temperature, fuel flow, air ratio
- Compensates for fouling and load changes

D. Utilities and Offsites

- Steam distribution
- Cooling water networks
- Nitrogen and instrument air systems

4. DCS in Relation to AI/ML

DCS delivers the operational data stream that enables AI/ML analytics

DCS Function	AI/ML Enhancement	Engineering Benefit
Real-time data acquisition	**ML models** detect patterns	Early anomaly detection
Alarm management	**NLP** analyzes operator logs	Better safety insights
Control loops	**Reinforcement learning** optimizes tuning	Adaptive control
Historian data	**Deep learning** predicts failures	Predictive maintenance
Operator support	**Decision engines** recommend actions	Smarter operation

Digital Plant: An industrial facility in which plant data, automation, process models, AI, digital twins, and decision-support systems are integrated.

Digital Twin: A continuously updated virtual representation of a physical asset, process, or system. It may combine real-time sensor data, historical information, first-principles models, AI/ML algorithms, simulations, monitoring

systems, and operational feedback.

Example: A refinery digital twin may predict heat-exchanger fouling and recommend a suitable cleaning schedule.

Discriminator: The component of a Generative Adversarial Network that attempts to distinguish between actual data and data created by the generator.

Distributed Control System (DCS): A computerized control system used to monitor and regulate industrial processes. DCS data may be transferred to historians and AI models for analysis.

Dynamic Modeling: The mathematical representation of how process variables change with time.

Example: Modeling reactor temperature following a cooling-system failure.

Dynamic Principal Component Analysis (DPCA): A form of PCA that incorporates time-dependent relationships and is useful for monitoring dynamic industrial processes.

Dynamic Process Simulation: A process simulation that calculates how process conditions change over time. It is useful for startup, shutdown, control-system testing, equipment failure, emergency response, and operator training.

E

Early-Warning System: A monitoring system designed to identify a developing abnormal condition before it becomes hazardous or causes equipment failure.

Emotional Intelligence: The ability to recognize, understand, and manage one's own emotions while responding appropriately to the emotions of others. It supports leadership, teamwork, communication, and conflict management.

Emotional Intelligence (EI): is the capability to understand, manage, and use emotions—your own and those of others—to guide thinking, behaviour, and decision-making. In modern engineering practice, EI is no longer optional. It is a **core competency** that determines how effectively engineers lead teams, collaborate, communicate, innovate, and navigate complexity.

This is a structured explanation of Emotional Intelligence within the Human-Centered Skills framework.

1. The Role of Emotional Intelligence in Professional Performance

EI consists of four interconnected abilities:

- **Self-Awareness** — recognising your emotions and their impact
- **Self-Management** — regulating emotions to stay composed and effective
- **Social Awareness** — understanding others' emotions, motivations, and perspectives
- **Relationship Management** — building trust, resolving conflict, and inspiring others

These are the *human* skills that complement AI, automation, and technical expertise.

2. The Role of Emotional Intelligence in Engineering Performance

EI is not "soft"—it is **strategic**.

- Engineers with high EI communicate more clearly
- They lead teams with less friction and more trust
- They make better decisions under pressure
- They adapt faster to change
- They collaborate more effectively across disciplines

In a world where AI handles computation, EI handles **coordination, leadership, and human judgment**.

3. EI + AI: A Powerful Partnership

AI amplifies technical capability. EI amplifies human capability.

Together, they create the modern engineer:

- AI processes data → EI interprets impact
- AI predicts outcomes → EI guides decisions
- AI automates tasks → EI motivates teams
- AI optimizes systems → EI optimizes people

This is the essence of **Human-Centered Engineering**.

4. EI in the Refinery, CPI, and Industrial Practice

Emotional Intelligence directly improves:

- **Safety culture** — people speak up, listen, and respond constructively
- **Shift-team communication** — fewer misunderstandings, better handovers
- **Crisis management** — calm leadership during upsets or emergencies
- **Cross-functional collaboration** — operations, maintenance, and engineering alignment
- **Innovation** — psychological safety encourages new ideas

EI is the “hidden variable” behind high-performing industrial teams.

5. EI Skills Engineers Can Build Today

Each item includes a Guided Link for deeper exploration.

- **Active Listening** — understanding before responding
- **Empathy** — seeing situations from others’ perspectives
- **Constructive Communication** — clarity without conflict
- **Emotional Regulation** — staying steady under pressure
- **Influence and Motivation** — inspiring action without authority

These are the skills that AI cannot replace.

6. Summary

Emotional Intelligence is the **human operating system** of modern engineering.

It enables:

- Better leadership
- Better collaboration
- Better decisions
- Better innovation

- Better safety

And when combined with AI, EI becomes the differentiator that elevates engineers from technical contributors to **strategic leaders**.

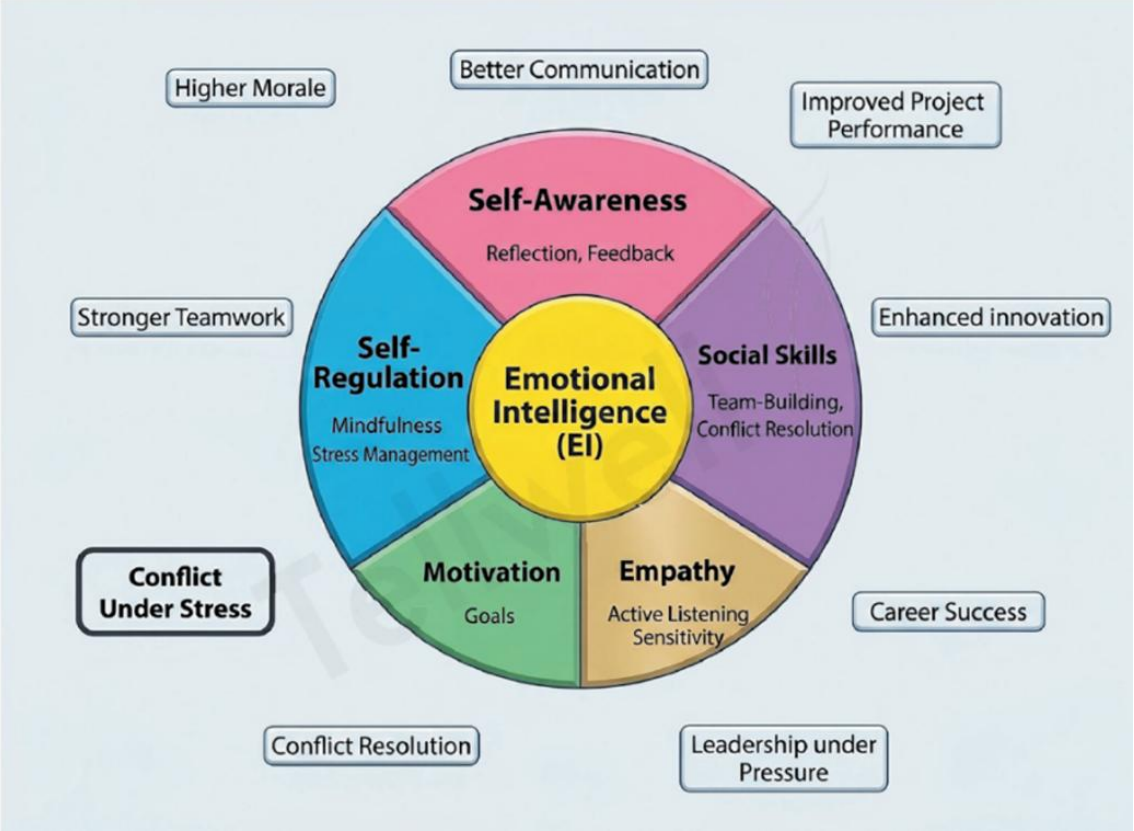


Figure 16. Emotional Intelligence in Engineering – Components to Outcomes.

Energy Integration: is the systematic approach to optimising energy use across process units recovering, reusing, and redistributing heat and power to minimise waste and improve efficiency. It is a cornerstone of sustainable process design and a key enabler of AI-driven optimisation in modern plants (See Figure 17).

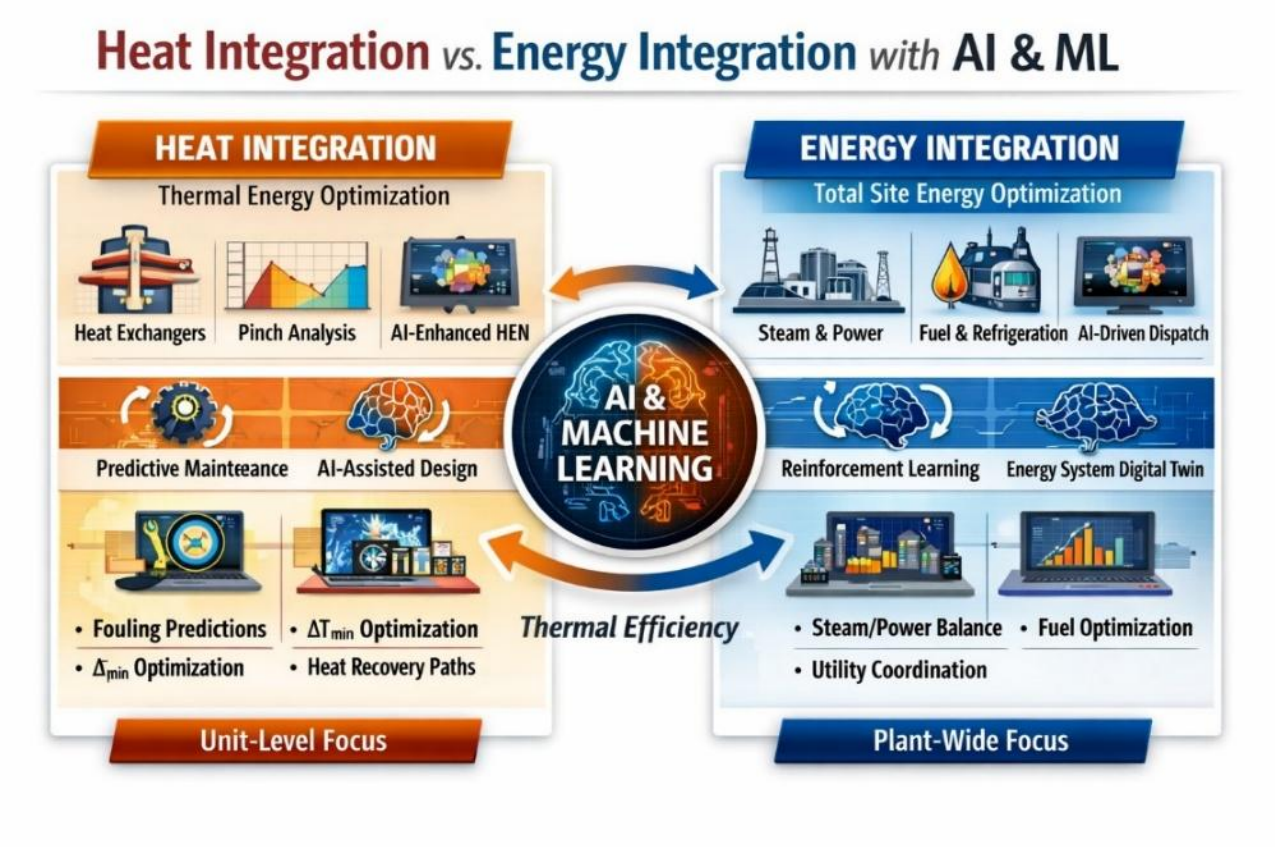


Figure 17: AI-Driven Heat and Energy Integration: From Thermal Efficiency to Total Site Optimisation (Source: Author's illustrative visualization developed with AI-assisted tools.)

1. Core Concept

Energy Integration focuses on **maximising thermal efficiency** by linking hot and cold streams through **heat-exchange networks**. It aims to reduce external utilities (steam, fuel, cooling water) by internal energy recovery.

- **Pinch Analysis** — identifies minimum energy targets and optimal heat-exchange matches

- **Heat Exchanger Network (HEN)** — designs the physical system for energy recovery
- **Process Integration** — extends the concept to mass and utility systems

2. Role of AI in Energy Integration

AI enhances Energy Integration by enabling:

AI Function	Application in Energy Integration
Predictive analytics	Forecasts heat-load variations and optimises exchanger performance
Machine learning models	Detects inefficiencies and suggests reconfiguration of HENs
Digital twins	Simulates plant-wide energy flows for real-time optimisation
Reinforcement learning	Adjusts control strategies dynamically to maintain pinch targets
AI-assisted design tools	Automates exchanger network synthesis and retrofit planning

AI transforms Energy Integration from static design to **adaptive, intelligent optimisation**.

3. Benefits in Petroleum and Petrochemical Operations

- **Reduced fuel consumption** and CO_2 emissions
- **Improved process efficiency** and profitability
- **Enhanced reliability** through predictive maintenance
- **Dynamic optimisation** under varying feed and product conditions
- **Integration with sustainability goals** and net-zero pathways

4. Example Applications

- **Crude preheat trains** — AI optimises exchanger cleaning schedules and heat recovery
- **Steam networks** — predictive control balances generation and demand
- **Reformer and cracker units** — AI identifies energy bottlenecks and retrofit opportunities

- **Utility systems** — integrated AI models coordinate steam, cooling, and power systems

5. Human-Centered Leadership in Energy Integration

Leadership ensures that AI-driven energy strategies align with:

- **Safety and reliability standards**
- **Ethical and environmental commitments**
- **Cross-disciplinary collaboration** between process, control, and sustainability teams

This is where **Leadership** and **Human-Centered Skills** merge with technical innovation.

6. Summary

Energy Integration is the **bridge between efficiency and sustainability**. AI provides the intelligence; engineers provide the judgment. Together, they create **smart, resilient, and low-carbon petroleum and petrochemical operations**.

Ethical judgment: is the ability to make decisions that are **responsible, fair, transparent, and aligned with professional and societal values**, especially when the stakes are high and the answers are not obvious. In engineering today

where AI, automation, and globalized operations shape daily work, ethical judgment has become a **core leadership competency**.

1. The Role of Ethical Judgment in Professional Engineering Conduct

Ethical judgment is the disciplined process of deciding **what ought to be done**, not just what *can* be done. It involves:

- **Moral awareness** — recognising when a situation has ethical implications
- **Moral reasoning** — evaluating options using principles, values, and consequences
- **Professional responsibility** — acting in accordance with codes of practice (AIChE, IChemE, NSPE)
- **Courage and integrity** — doing the right thing even when it is difficult

Ethical judgment is the **anchor** that keeps engineering decisions grounded in safety, fairness, and public trust.

2. The Importance of Ethical Judgment in Engineering

Ethical judgment is not abstract; it is **practical** and **operational**.

Engineers routinely face decisions involving:

- Safety vs. production
- Cost vs. environmental impact
- Innovation vs. risk
- Transparency vs. organisational pressure
- AI recommendations vs. human oversight

Ethical judgment ensures that decisions protect:

- **People**
- **The environment**
- **The public**
- **The profession**
- **The organisation's long-term credibility**

3. Ethical Judgment in the Age of AI

AI introduces new ethical dimensions:

- **Bias in algorithms**
- **Transparency of AI recommendations**

- **Accountability for automated decisions**
- **Data privacy and security**
- **Human oversight of AI-driven operations**

This is why engineers must combine:

- **AI capability**
- **Human-centred skills**
- **Ethical reasoning**

AI can optimise, but **ethical judgment decides whether the optimisation is acceptable**.

4. Ethical Judgment in Refinery and CPI Operations

Ethical judgment directly influences:

- **Process safety** — choosing safety over shortcuts
- **Environmental stewardship** — emissions, waste, energy use
- **Incident reporting** — honesty and transparency
- **Maintenance decisions** — avoiding deferred maintenance risks
- **AI-assisted operations** — ensuring human review and accountability

Examples of ethical dilemmas:

- Should production be increased when a known equipment issue exists?
- Should an AI recommendation be followed if it conflicts with operator intuition?
- Should a near-miss be reported even if it may reflect poorly on the team?

Ethical judgment guides the right answer.

5. Skills That Strengthen Ethical Judgment

Each item highlights a core element of ethical judgment for deeper understanding.

- **Critical thinking** — analysing consequences and trade-offs
- **Emotional intelligence** — understanding human impact
- **Courageous communication** — speaking up when needed
- **Systems thinking** — seeing the broader implications
- **Values-based leadership** — aligning decisions with principles

These skills ensure engineers act not only with intelligence, but with **wisdom**.

6. Summary

Ethical judgment is the **moral compass** of engineering. It ensures that:

- AI is used responsibly
- Safety is never compromised
- Decisions reflect integrity
- Engineering remains a trusted profession

In a world where AI accelerates decision-making, ethical judgment ensures those decisions remain **human, principled, and worthy of public trust**.

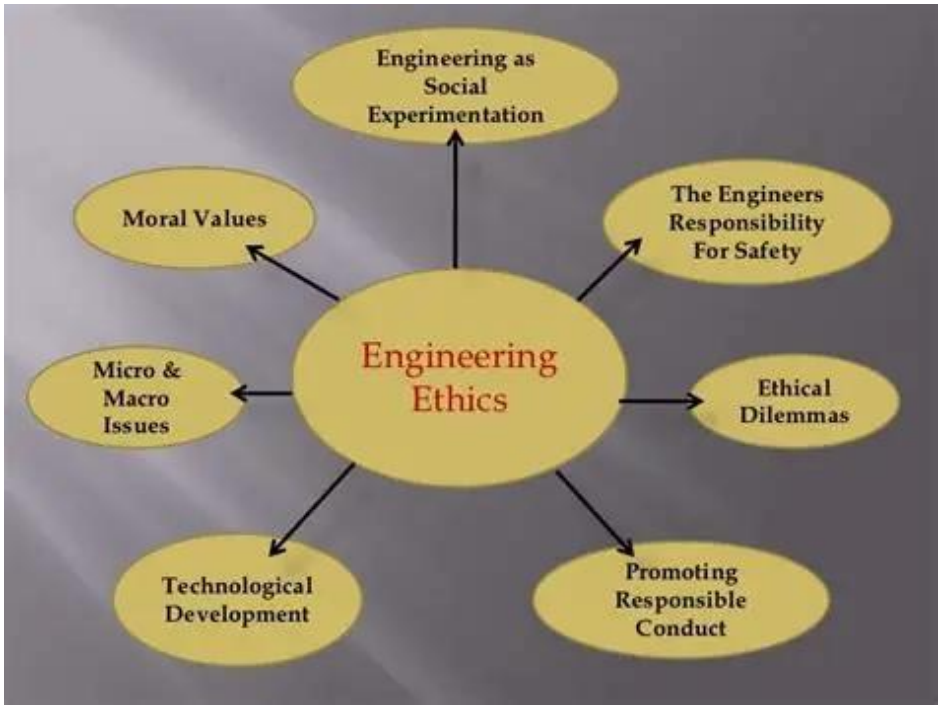


Figure 18a. Engineering Ethics (Source: Author's illustrative visualization developed with AI-assisted tools.)

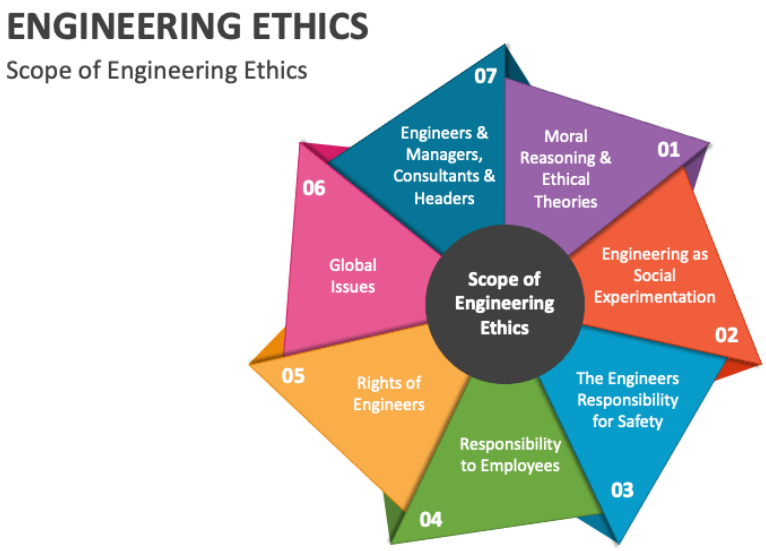


Figure 18b. Scope of Engineering Ethics (Source: Author's illustrative visualization developed with AI-assisted tools.)

Generative Artificial Intelligence (AI): a. Generative AI is a branch of Artificial Intelligence (AI) that can create or generate new content by learning patterns from existing data. **b**. Generative AI is an intelligent system capable of creating new information, ideas, solutions, or content from learned data patterns. Generative AI learns from large amounts of information and then produces new outputs that resemble human-created work.

Why Generative AI is considered a Deep Learning subset

Generative AI relies on **deep neural networks**, especially:

- **Transformers** (e.g., GPT-type models)
- **Diffusion models** (e.g., Stable Diffusion)
- **GANs** (Generative Adversarial Networks)
- **VAEs** (Variational Autoencoders)

All of these are **deep learning architectures**, meaning they use multi-layer neural networks trained on massive datasets.

So generative AI is not just "part of deep learning" — it is one of the most advanced *applications* of deep learning.

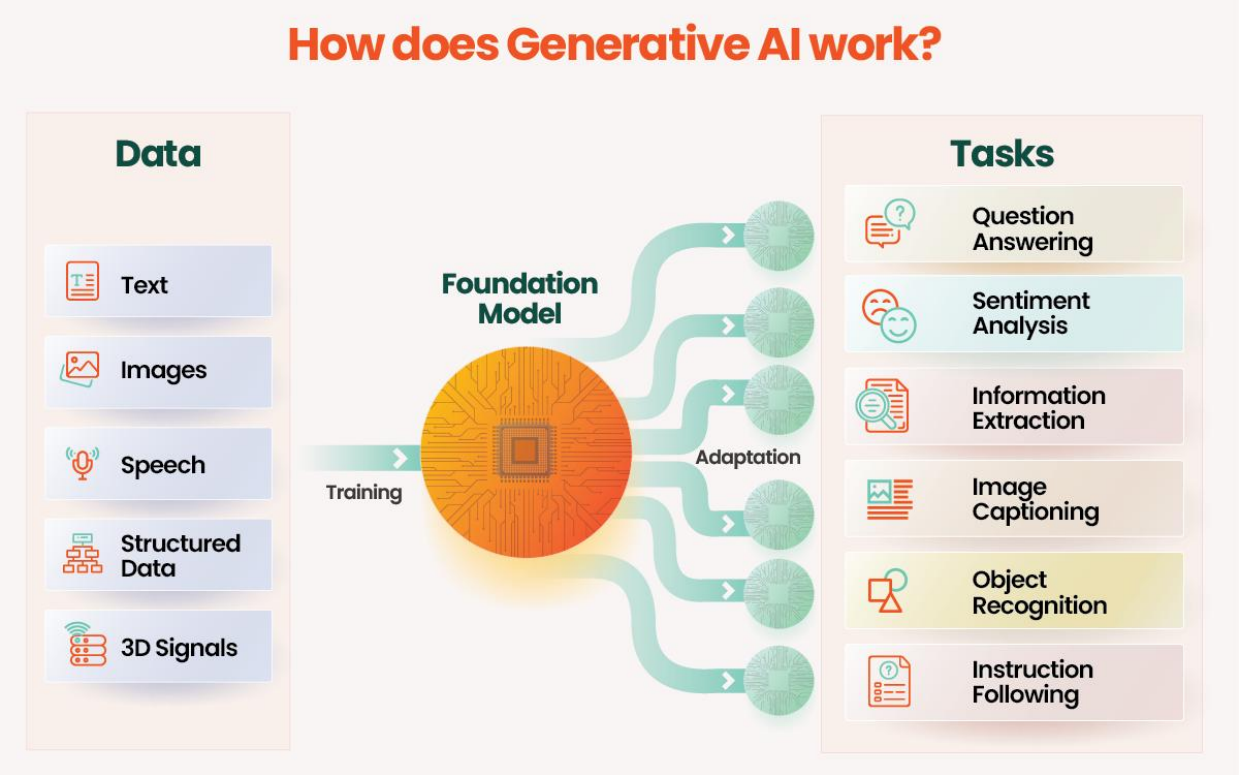


Figure 19a. Generative AI application

Generative AI within the AI hierarchy

The modern AI stack is typically structured like nested boxes:

- **Artificial Intelligence (AI)** Broadest category — any system that mimics human intelligence.
- **Machine Learning (ML)** Subset of AI — systems that learn patterns from data.
- **Deep Learning (DL)** Subset of ML — neural networks with many layers.

- **Generative AI (GenAI)** Subset of DL — models that *create* new content (text, images, audio, code, etc.) based on learned patterns.

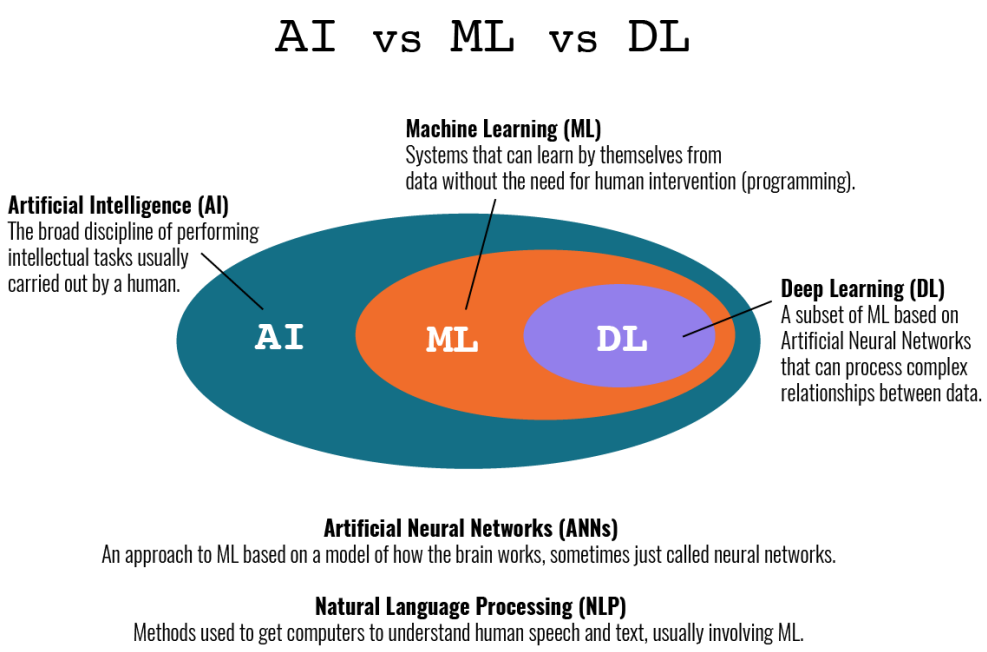


Figure 19b. AI vs. ML vs. DL



Figure 19c Generative Artificial Intelligence brain for process engineering

(Source: Author's illustrative visualization developed with AI-assisted tools.)



Figure 19d. Generative AI brain with Neuron and ANN for process engineering (Source: Author's illustrative visualization developed with AI-assisted tools.)

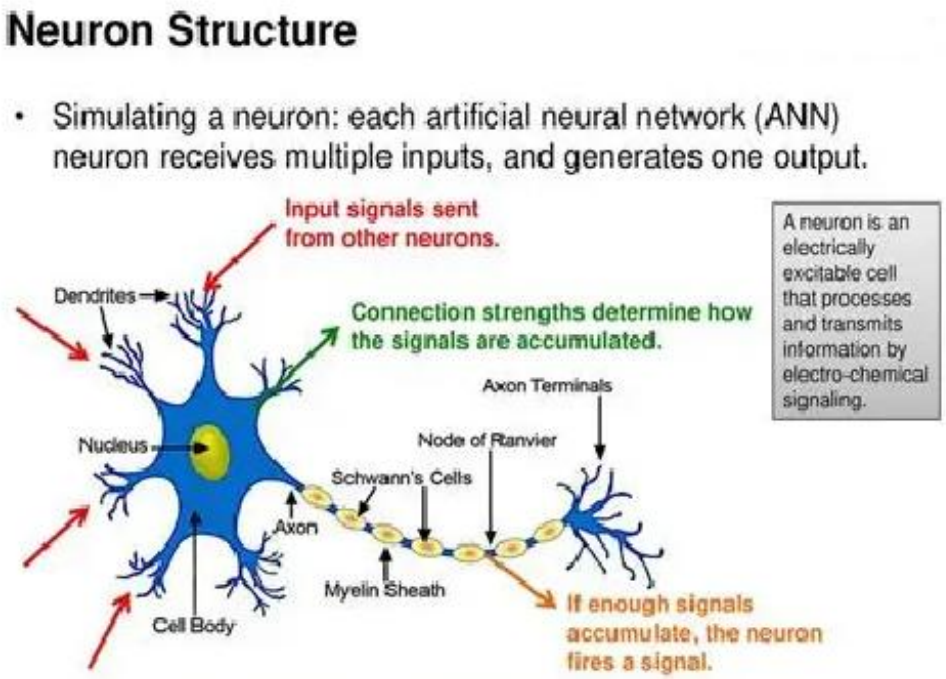


Figure 19e. Neuron Structure (Source: Illustrative AI-assisted engineering visualization.)

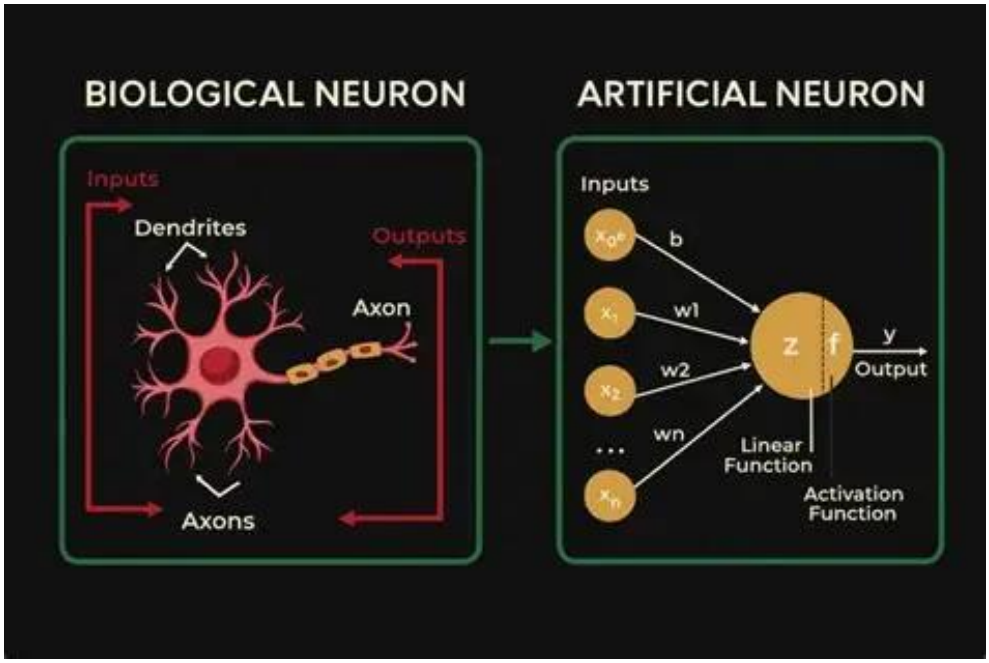


Figure 19f. Biological Neuron vs. Artificial Neuron (Source: Illustrative AI-assisted engineering visualization.)

Generative Adversarial Networks (GAN): is a class of **generative models** that learns to create new data by setting up a **competition** between two neural networks:

- **Generator** — creates synthetic data
- **Discriminator** — evaluates whether the data is real or fake

These two networks train **against each other** in a process called *adversarial learning*. The generator improves until it can produce data that is **indistinguishable from real data**.

GANs are inspired by the **brain's ability to imagine, refine, and evaluate possibilities**, similar to how engineers iterate designs.

Hazard and Operability Study (HAZOP): is a systematic, structured, team-based method used to identify potential hazards and operability problems in chemical and process systems. It examines how a process might deviate from its intended design and what consequences could arise.

HAZOP is one of the most widely used process safety analysis tools in the chemical and petrochemical industries.

1. Core Purpose of HAZOP

- Identify **hazards** (fire, explosion, toxicity, runaway reactions)
- Identify **operability issues** (startup problems, shutdown risks, equipment failures)
- Understand **causes, consequences, safeguards, and recommendations**
- Improve **design, procedures, instrumentation, and human factors**

2. The Operation of HAZOP in Process Analysis

HAZOP uses **guide words** to explore deviations from normal operation.

Common Guide Words

- **No** (no flow, no pressure)

- **More** (more temperature, more level)
- **Less**
- **Reverse**
- **As well as**
- **Other than**

Each deviation is analyzed for:

- **Causes**
- **Consequences**
- **Existing safeguards**
- **Recommendations**

3.. HAZOP Examples for Chemical/Process Engineers

A. Distillation Column

- **Deviation:** More pressure
- **Cause:** Condenser fouling
- **Consequence:** Relief valve lift, potential overpressure
- **Safeguard:** Pressure control loop

- **Recommendation:** Add high-pressure alarm

B. Reactor

- **Deviation:** More temperature
- **Cause:** Cooling water failure
- **Consequence:** Runaway reaction
- **Safeguard:** High-temperature trip
- **Recommendation:** Redundant cooling system

C. Pumping System

- **Deviation:** No flow
- **Cause:** Pump trip or suction blockage
- **Consequence:** Reactor starvation, cavitation
- **Safeguard:** Low-flow alarm
- **Recommendation:** Install suction strainer

4. HAZOP in Relation to AI/ML

AI/ML enhances HAZOP by analyzing **large volumes of historical and real-time data**.

HAZOP Element	AI/ML Enhancement	Engineering Benefit
Deviations	**Anomaly detection**	Early detection of abnormal behaviour
Causes	**Machine learning** identifies root-cause patterns	Faster troubleshooting
Consequences	**Predictive models** simulate outcomes	Better risk assessment
Safeguards	**Digital twins** test safeguard performance	Improved reliability
Recommendations	**NLP** analyzes past incident reports	Smarter recommendations

AI does **not** replace HAZOP — it **augments** it by providing deeper insights and data-driven evidence.

Heat Integration: is the systematic method of **recovering, reusing, and redistributing heat within a process** to minimise external energy consumption. It is one of the most powerful tools for improving refinery and petrochemical plant efficiency, reducing fuel use, lowering CO_2 emissions, and enhancing profitability (See Figure 17).

1. The Basis of Heat Integration in Modern Process Engineering

Heat Integration focuses on designing processes so that **hot streams** (that need cooling) transfer heat to **cold streams** (that need heating), reducing the need for:

- Fired heaters
- Steam generation
- Cooling water
- Refrigeration

It is the foundation of **Process Integration** and is typically implemented through:

- **Pinch Analysis**
- **Heat Exchanger Networks (HEN)**
- **Composite Curves**

2. The Importance of Heat Integration in Refineries and Petrochemical Plants

Heat Integration directly improves:

- **Energy efficiency** (10–35% reduction in utility use is common)

- **Fuel consumption** (lower furnace duty)
- **CO_2 emissions** (less combustion)
- **Operating costs** (steam and fuel savings)
- **Process reliability** (better temperature control)

It is especially impactful in:

- Crude distillation units (CDU)
- Hydroprocessing units
- Steam crackers
- Aromatics complexes
- Polymer plants

Energy Balance: A first-principles equation based on conservation of energy. It accounts for energy entering, leaving, accumulating, being generated, or being consumed within a system.

Energy Integration: The coordinated optimization of process heat, steam, electricity, fuel, cooling water, and other utility systems across a facility (See Figure 17).

Engineering Judgment: The application of technical knowledge, experience, context, standards, ethics, and professional responsibility to make sound engineering decisions.

Equipment Health Monitoring: The assessment of machinery or equipment condition using operating and condition-monitoring data.

Expert System: An AI system that uses stored rules and specialist knowledge to provide recommendations or solve problems within a defined area.

Explainability: The extent to which the factors or reasoning behind a model's prediction can be understood.

F

Fault Detection: The identification of equipment, instrument, or process malfunctions.

Example: Detecting an abnormal pump-vibration pattern indicating cavitation or bearing deterioration.

Feature: An input variable used by a machine-learning model.

Example: Feed temperature, pressure, reflux ratio, composition, and tray efficiency are features in a distillation-purity model.

Feed Composition: The concentration or fraction of components entering a process unit. Changes in feed composition can significantly affect product quality and operating behaviour.

First-Order Kinetics: A reaction-rate relationship in which the reaction rate is proportional to the concentration of one reactant.

First-Principles Model: A mathematical model derived from fundamental engineering laws, including mass balances, energy balances, thermodynamics, reaction kinetics, fluid flow, heat transfer, and phase equilibrium.

Fluid Catalytic Cracking (FCC): A refinery process that converts heavy gas oils into lighter products such as gasoline, LPG, and olefins using a circulating catalyst.

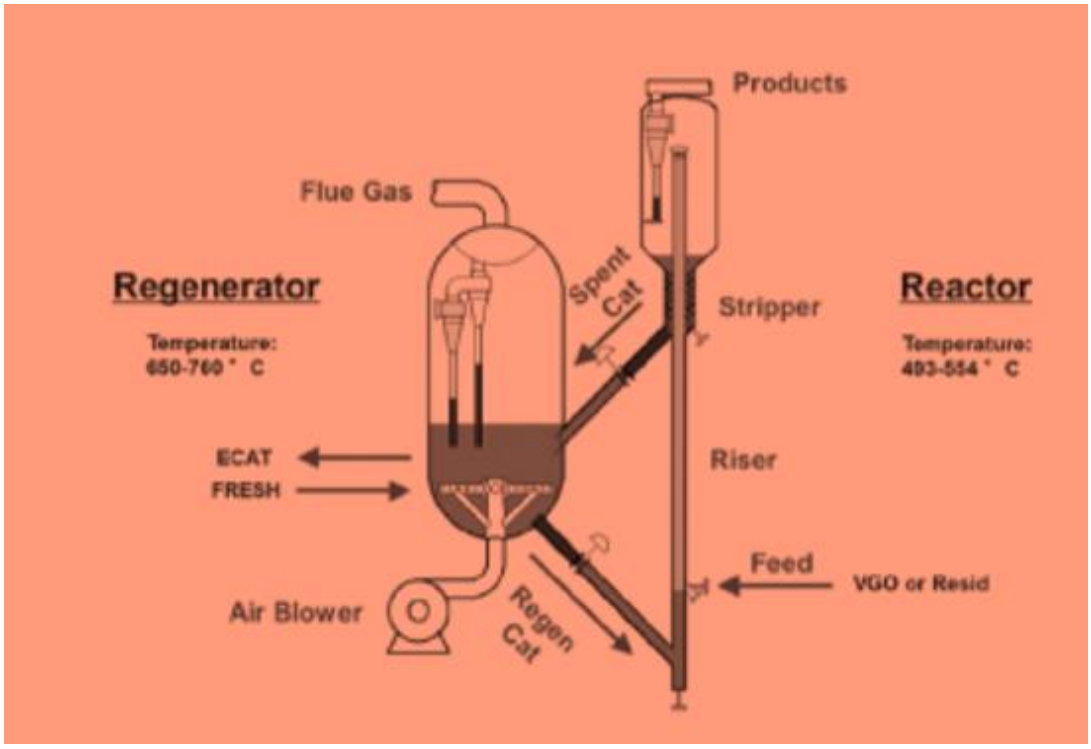


Figure 20. Fluidized bed catalytic cracking (FCC) unit

Forget Gate: The LSTM component that determines which previously stored information should be discarded.

Fouling: The accumulation of deposits on equipment surfaces, causing reduced heat transfer, increased pressure drop, or restricted flow.

Example: AI may forecast heat-exchanger fouling and support cleaning-schedule optimization.



Figure 21. A fouled shell and tube heat exchanger

G

Gated Memory Architecture: The structure used by LSTM networks to control how information is stored, updated, passed forward, or forgotten.

Gaussian Process: A probabilistic machine-learning model that may be used as a surrogate model for predicting process behaviour and estimating uncertainty.

Generative Adversarial Network (GAN): A generative deep-learning model containing two competing neural networks: a generator and a discriminator.

The generator creates synthetic data, while the discriminator attempts to distinguish generated data from actual data.

Example: A GAN may generate realistic examples of rare reactor-runaway trajectories for training and model stress-testing.

Generative Artificial Intelligence (Generative AI or GAI): AI systems capable of creating new text, code, images, designs, process alternatives, procedures, data, or other content based on patterns learned from existing information.

Generator: The component of a GAN that produces synthetic samples intended to resemble the original training data.

Global Warming Potential (GWP): A measure of how much heat a greenhouse gas traps in the atmosphere relative to carbon dioxide over a specified period.

Green Hydrogen: Hydrogen manufactured by splitting water through electrolysis using electricity generated from renewable sources such as wind, solar, or hydroelectric power.

$$2H_2O \rightarrow 2H_2 + O_2$$

Example: A water electrolyzer powered by an offshore wind farm may produce green hydrogen for refining, ammonia manufacture, or energy storage.

Greenhouse Gases (GHGs): Atmospheric gases that absorb and re-emit infrared radiation, thereby contributing to the greenhouse effect and climate change.

Important greenhouse gases include:

- Carbon dioxide
- Methane
- Nitrous oxide
- Hydrofluorocarbons
- Perfluorocarbons
- Sulfur hexafluoride
- Nitrogen trifluoride

Example: Carbon dioxide from refinery furnaces and methane released from natural-gas systems both contribute to greenhouse-gas emissions.

Grey Hydrogen: Hydrogen produced from fossil fuels, most commonly natural gas through steam methane reforming, without capturing the resulting carbon dioxide emissions.

Simplified steam methane reforming reaction:

$$CH_4 + H_2O \rightarrow CO + 3H_2$$

Water-gas shift reaction:

$$CO + H_2O \rightarrow CO_2 + H_2$$

Example: A refinery steam methane reformer operating without carbon capture generally produces grey hydrogen.

H

Hazard Analysis: A structured examination of process hazards, their causes, consequences, safeguards, and risk-reduction measures.

Hazard and Operability Study (HAZOP): A structured, multidisciplinary method used to identify deviations from the intended design or operation of a process and evaluate their causes, consequences, safeguards, and recommended actions.

Common HAZOP guide words include:

- No

- More
- Less
- Reverse
- As well as
- Other than
- Part of

These guide words are applied to process parameters such as flow, pressure, temperature, level, composition, and reaction.

Example: Applying “No Flow” to an exothermic reactor’s cooling-water supply may identify loss of cooling, rising temperature, accelerated reaction, pressure increase, and possible thermal runaway.

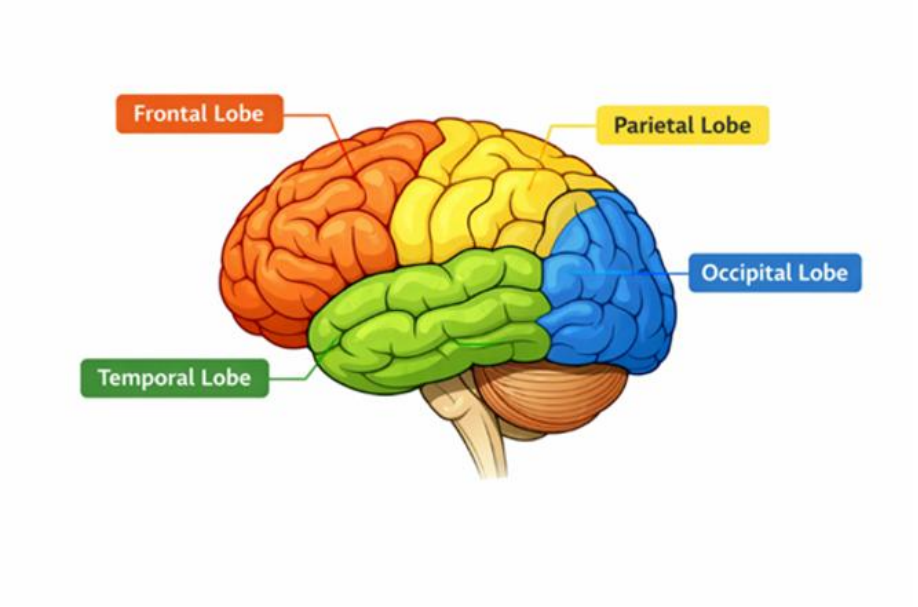
Heat Integration: The recovery and reuse of heat between process streams to reduce external heating and cooling requirements (See Figure 19).

Hidden Layer: A neural-network layer positioned between the input and output layers. Hidden layers transform input data and learn complex relationships.

Historian: An industrial database that continuously collects, stores, compresses, and organizes time-dependent process data.

Human Brain – The Biological Model: The biological organ responsible for cognition, perception, memory, learning, movement, emotion, communication, reasoning, and control of vital functions. The Biological model is a **complex network of neurons** that processes sensory input, stores information, and makes decisions through **learning and adaptation**.

Its key functions: **perception**, **memory**, **pattern recognition**, **decision-making**, and **learning** mirror the computational principles behind AI and ML.



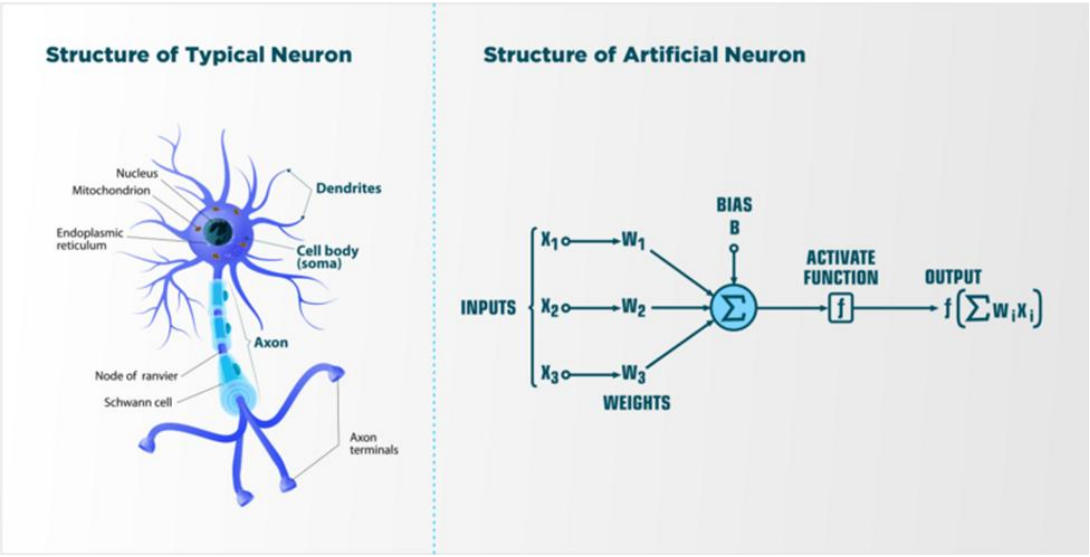


Figure 22. Human brain and structures of typical neuron and Artificial neuron (Source: illustrative visualization developed with AI-assisted tools.)

Human Centered Competencies: are the essential interpersonal, cognitive, ethical, and leadership skills that enable engineers to work effectively with people, technology, and complex systems. They represent the uniquely human capabilities that AI cannot replace, but AI can amplify.

These competencies ensure that engineers remain effective decision-makers, communicators, collaborators, and leaders in an AI-enabled world.

Core Human-Centered Competencies

A. Communication: The ability to convey ideas clearly across disciplines, cultures, and roles. Includes listening, reporting, presenting, and translating technical insights.

B. Critical Thinking: Evaluating information, questioning assumptions, and making sound judgments, especially when interpreting AI/ML outputs.

C. Collaboration and Teamwork: Working effectively with operators, managers, data scientists, and cross-functional teams.

D. Ethics and Professional Responsibility: Ensuring safe, transparent, and responsible use of technology and data.

E. Leadership: Guiding teams through digital transformation, influencing decisions, and fostering trust.

F. Creativity and Innovation: Generating new ideas, solving novel problems, and designing better systems.

G. Situational Awareness: Understanding the plant environment, anticipating risks, and recognizing abnormal conditions.

H. Adaptability and Lifelong Learning: Staying current with evolving technologies, methods, and industry expectations.

Human-Centered Skills: The interpersonal, cognitive, ethical, and leadership abilities required for effective engineering practice. They include communication, teamwork, critical thinking, creativity, emotional intelligence, leadership, empathy, and responsibility.

Human Intelligence: The natural ability to understand context, reason, learn, communicate, create, exercise judgment, consider ethics, and accept responsibility.

Hybrid AI Model: A model that combines first-principles engineering with data-driven AI or ML.

Example: A process simulator may calculate a base prediction, while an ML model corrects the prediction using actual plant data.

Hydrogen Manufacture: The industrial production of hydrogen from water, hydrocarbons, biomass, geological sources, refinery off-gases, or other feedstocks.

Major production routes include:

- Steam methane reforming
- Autothermal reforming
- Partial oxidation
- Coal or biomass gasification
- Water electrolysis
- Methane pyrolysis
- Refinery off-gas recovery

- Natural or geological hydrogen extraction

Hydrogen is used in:

- Hydrotreating
- Hydrocracking
- Ammonia manufacture
- Methanol manufacture
- Fuel cells
- Synthetic-fuel production
- Petroleum-product upgrading

Hydrogen Purification: The removal of impurities such as carbon dioxide, carbon monoxide, methane, water, nitrogen, and hydrogen sulfide from a hydrogen-rich gas.

Common purification methods include:

- Pressure swing adsorption
- Membrane separation
- Solvent absorption
- Cryogenic separation
- Adsorption and drying

Hydrogen-Consumption Optimization: The use of engineering models or AI to minimize hydrogen use while maintaining product quality, catalyst protection, and process safety in hydroprocessing units.

I

Independent Component Analysis (ICA): A statistical method used to separate multivariable data into components that are as independent as possible. It may assist fault detection and process monitoring.

Industrial Internet of Things (IIoT): A network of industrial sensors, instruments, equipment, software, and data systems that communicate and exchange operating information.

Industry 4.0: **a**. The integration of automation, digital technologies, AI, IIoT, analytics, robotics, cloud computing, and intelligent manufacturing. **b**. refers to the fourth industrial revolution, characterized by the integration of digital technologies, automation, AI/ML, data analytics, and cyber-physical systems into manufacturing and process industries.

It transforms traditional plants into smart, connected, autonomous systems capable of real-time optimization, predictive intelligence, and seamless human–machine collaboration.

1. Core Pillars of Industry 4.0

- **Cyber-Physical Systems (CPS)** — physical equipment integrated with digital intelligence
- **Internet of Things (IoT)** — sensors and devices connected across the plant
- **Big Data and Analytics** — high-volume data processed for insights
- **Artificial Intelligence and Machine Learning** — predictive models, optimization, automation
- **Cloud and Edge Computing** — scalable computing power close to the process
- **Digital Twins** — virtual replicas of equipment and processes
- **Autonomous Systems** — self-optimizing, self-correcting operations

Industry 4.0 is the **digital backbone** of modern engineering.

Inference Algorithm: A computational method that uses available data or rules to draw conclusions or make predictions.

Input Gate: The LSTM component that determines what new information should be stored in memory.

Input Layer: The first layer of an ANN, where process variables or features enter the model.

Instrument Error: A measurement difference caused by calibration problems, drift, malfunction, installation conditions, or other instrument limitations.

Intelligent Manufacturing: The use of connected sensors, automation, AI, data analytics, robotics, and digital systems to improve production performance.

Intelligent Monitoring: refers to the use of AI/ML, advanced analytics, smart sensors, and automated reasoning to continuously observe, interpret, and predict the behaviour of industrial processes, equipment, and safety systems.

Unlike traditional monitoring which is reactive and threshold-based, intelligent monitoring is:

- **Predictive** (foresees issues before they occur)
- **Adaptive** (learns from new data)
- **Context-aware** (understands process relationships)

- **Autonomous** (acts or recommends actions in real time)

It transforms raw data into **actionable intelligence**.

1. Core Capabilities of Intelligent Monitoring

- **Real-time Data Fusion** — combining sensor, historian, and operator data
- **Anomaly Detection** — identifying abnormal patterns before alarms trigger
- **Predictive Analytics** — forecasting failures or deviations
- **Condition Monitoring** — tracking equipment health continuously
- **Root-Cause Reasoning** — diagnosing why deviations occur
- **Automated Alerts and Recommendations** — guiding operators with intelligent insights

Intelligent monitoring is the **brain** of modern industrial operations.

2. Intelligent Monitoring in Chemical/Process Engineering

A. Equipment Health Monitoring

AI models analyze vibration, acoustic, thermal, and pressure data to detect:

- Pump cavitation
- Compressor surge precursors
- Heat exchanger fouling
- Valve stiction

Outcome: Predictive maintenance and reduced downtime

B. Process Deviation Detection

Intelligent monitoring identifies subtle deviations long before alarms activate:

- Distillation column flooding indicators
- Reactor temperature drift
- Abnormal flare behaviour
- Utility system imbalances

Outcome: Early intervention and safer operations

C. Safety and Risk Monitoring

AI + NLP analyze:

- Alarm floods
- Operator logs

- Incident reports
- Safety system activations

Outcome: Improved situational awareness and risk reduction

D. Environmental and Emissions Monitoring

Smart sensors + ML track:

- VOC emissions
- Flare efficiency
- Fugitive leaks
- Wastewater quality

Outcome: Regulatory compliance and sustainability

E. Digital Twin Integration

Digital twins simulate process behaviour and compare it with real-time data to:

- Detect deviations
- Predict failures
- Recommend optimal actions

Outcome: Smarter, more adaptive operations

Intelligent Process Control: A control approach that incorporates AI, ML, optimization, adaptive models, or advanced analytics to improve process performance.

Isothermal CSTR: A Continuous Stirred Tank Reactor modeled under the assumption that reactor temperature remains constant.

J

Jacketed CSTR: A Continuous Stirred Tank Reactor surrounded by a jacket through which heating or cooling fluid flows to regulate reactor temperature.

Judgment: The human ability to evaluate technical evidence, uncertainty, context, safety, ethics, and consequences before selecting an action.

K

Kernel Principal Component Analysis (KPCA): A nonlinear extension of PCA used to identify complex patterns that cannot be represented adequately by linear principal components.

Kinetics: The study of reaction rates and the factors influencing them, including temperature, concentration, pressure, and catalyst activity.

L

LASSO Regression: A regression technique that applies a penalty to model coefficients and can reduce some coefficients to zero, thereby assisting variable selection.

Latent Variable: A reduced or hidden representation derived from several correlated measured variables. PCA and PLS use latent variables.

Layer of Protection: An independent safeguard used to prevent an initiating event from developing into a hazardous consequence or to reduce the severity of that consequence.

Layer of Protection Analysis (LOPA): is a semi-quantitative risk assessment method used in process safety to evaluate whether existing independent protection layers (IPLs) are sufficient to reduce the risk of a hazardous event to an acceptable level.

LOPA sits between qualitative methods (like HAZOP) and quantitative risk analysis (QRA). It provides a structured way to:

- Identify hazardous scenarios
- Estimate the frequency of initiating events
- Evaluate the effectiveness of protection layers
- Determine whether additional safeguards are required

LOPA is widely used in chemical and petrochemical industries because it is **rigorous, repeatable, and defensible**.

1. Key Elements of LOPA

- **Initiating Event Frequency** — how often a hazard could occur
- **Independent Protection Layers (IPLs)*** — safeguards that prevent or mitigate the event
- **Probability of Failure on Demand (PFD)** — likelihood that an IPL fails
- **Consequence Severity** — impact if the event occurs
- **Risk Tolerance Criteria** — company or regulatory limits
- **Risk Gap** — difference between actual and acceptable risk

LOPA quantifies risk using a simple equation:

Risk = Initiating Event Frequency × PFD of IPLs × Consequence Severity

2. Examples for Chemical/Process Engineers

A. Reactor Overpressure Scenario

- **Initiating event:** Cooling water failure
- **IPLs:** High-pressure alarm, SIS trip, relief valve
- **Outcome:** LOPA determines whether the relief system + SIS provide enough protection

B. Distillation Column Flooding

- **Initiating event:** Reflux pump failure
- **IPLs:** Level control, high-level shutdown, operator response
- **Outcome:** LOPA checks if additional safeguards (e.g., pump redundancy) are needed

C. Pump Seal Failure Leading to Vapor Cloud

- **Initiating event:** Mechanical seal leak
- **IPLs:** Gas detectors, automatic isolation valves, operator intervention

- **Outcome:** LOPA evaluates whether the risk of a vapor cloud explosion is ALARP

D. Furnace Tube Rupture

- **Initiating event:** Loss of flow
- **IPLs:** Flow interlock, burner management system, operator action
- **Outcome:** LOPA determines if SIS SIL level is adequate*

Leadership: The ability to guide people, communicate direction, build trust, manage uncertainty, and take responsibility for outcomes.

Leadership in Modern Engineering Practice: Leadership is no longer defined by hierarchy or job title. In today's engineering world shaped by AI, digital transformation, global collaboration, and rapid change leadership is the ability to **influence, guide, and elevate people and systems toward meaningful outcomes**.

A Clear, Structured Overview of Leadership in Engineering Practice

Learning: The process of acquiring knowledge or improving performance through experience, data, feedback, or training.

Linear Regression: A statistical method that represents the relationship between an output and one or more input variables using a linear equation.

Logic Solver: The processing component of a Safety Instrumented System that receives sensor signals, applies protective logic, and sends commands to final control elements.

Long Short-Term Memory Network (LSTM): A specialized recurrent neural network designed to learn long-term relationships in sequential or time-series data.

Example: An LSTM may forecast compressor degradation from vibration and temperature trends. LSTM introduces a memory cell and three gates that regulate the flow of information:

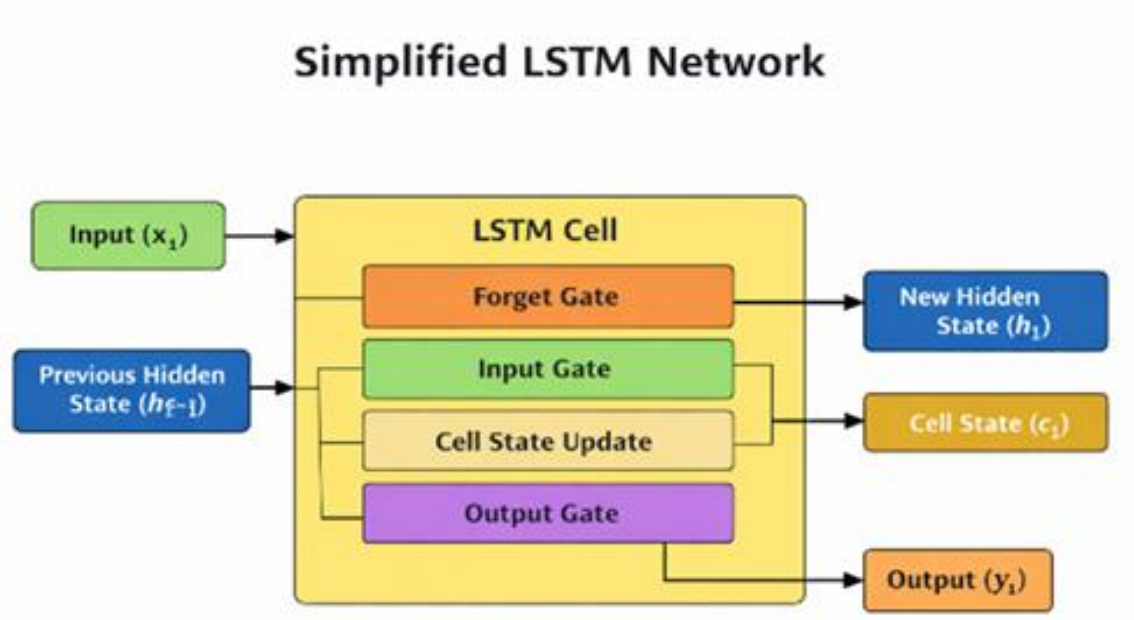


Figure 23. Simplified Long-Short Term Memory Network

Forget Gate: Decides which old information should be discarded

Input Gate: Determines what information should be stored in memory

Output Gate: Decides which information from memory should be passed to the next time step

Together, these gates allow the network to preserve important information for many time steps while discarding irrelevant information.

M

Machine Learning (ML): a. Is a subset of AI that enables computer systems to learn relationships and patterns from data without being explicitly programmed for every situation. **b**. ML is a branch of Artificial Intelligence in which computer systems learn patterns from data and improve their performance without being explicitly programmed.

Instead of following fixed rules, ML models:

- Analyze historical data
- Detect patterns and relationships
- Make predictions or decisions

- Continuously improve as more data becomes available

ML is the **engine** behind modern AI applications in engineering, safety, optimization, and automation.

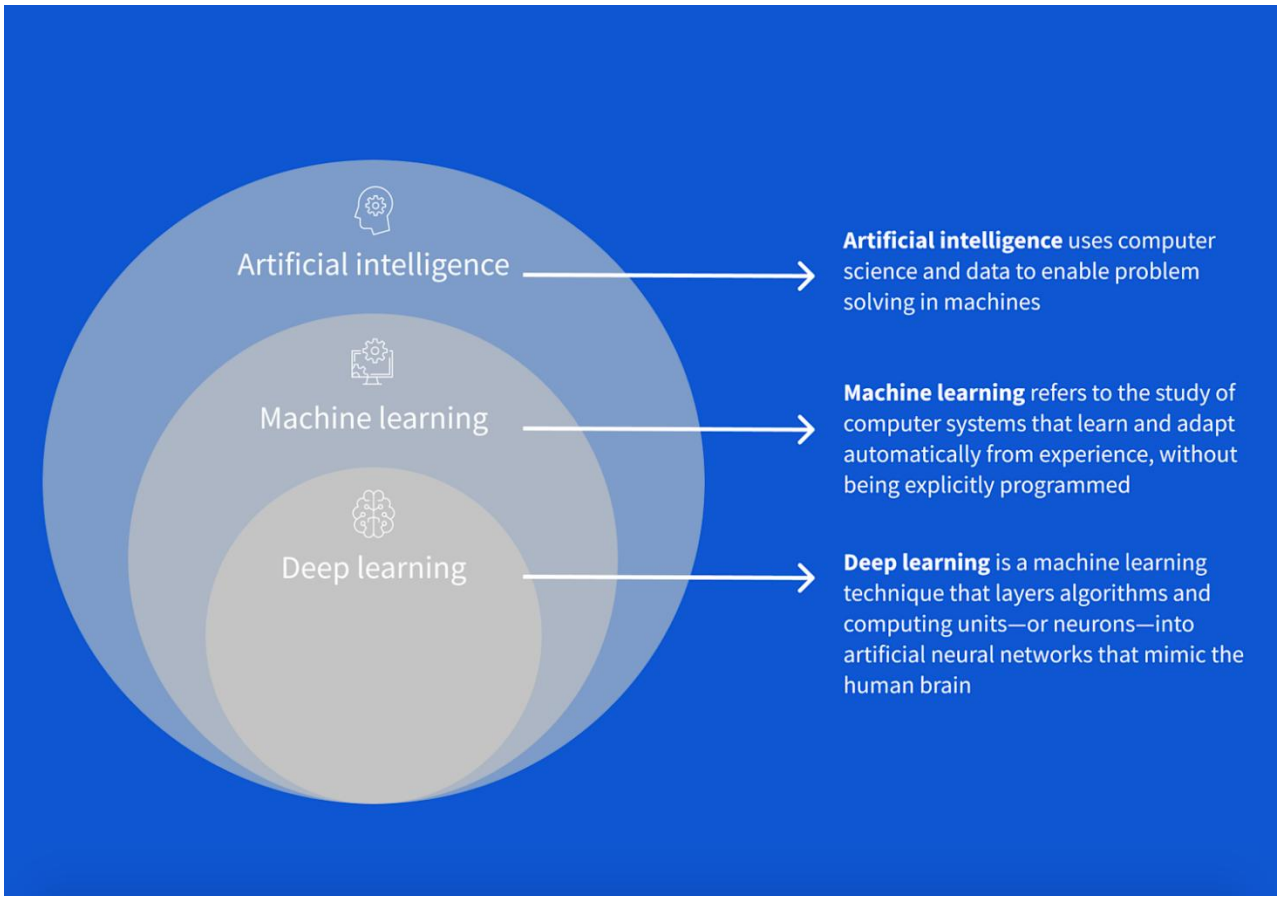


Figure 24. Deep Learning is a subset of Machine Learning, which is itself a subset of Artificial Intelligence.

1. Types of Machine Learning

A. Supervised Learning: The model learns from labeled examples (input → known output). Used for prediction and classification.

B. Unsupervised Learning: The model finds hidden patterns in unlabeled data. Used for clustering, anomaly detection, and feature extraction.

C. Reinforcement Learning: The model learns by interacting with an environment and receiving rewards or penalties. Used for control, optimization, and autonomous systems.

2. Machine Learning for Chemical/Process Engineers

ML is transforming process industries because plants generate **massive amounts of time-series, sensor, and operational data**.

Here are engineering-specific examples:

A. Predictive Maintenance: ML models analyze vibration, acoustic, and thermal data to predict equipment failures.

- Pumps
- Compressors
- Heat exchangers
- Turbines

Outcome: Reduced downtime and maintenance cost

B. Process Optimization: ML learns nonlinear relationships between variables such as temperature, pressure, flow, and composition.

- Optimizing reactor yield
- Reducing energy consumption in distillation
- Improving furnace efficiency

Outcome: Higher throughput and lower energy use

C. Fault Detection and Anomaly Recognition: ML identifies abnormal patterns before alarms occur.

- Distillation column flooding
- Reactor runaway indicators
- Compressor surge precursors

Outcome: Early warning and safer operations

D. Soft Sensors: ML estimates variables that are difficult or expensive to measure directly.

- Product purity
- Catalyst activity
- Viscosity or density

Outcome: Better monitoring and control

E. Safety and Incident Analysis: ML + NLP analyze:

- Operator logs
- Alarm histories
- Incident reports

Outcome: Improved risk awareness and prevention

F. Digital Twins: ML models simulate plant behaviour for:

- Training
- Scenario analysis
- Real-time optimization

Outcome: Smarter, more adaptive operations

3. ML + Cognitive Functions

Machine Learning mirrors key human cognitive functions:

Cognitive Function	ML Capability
Perception	Sensor data interpretation
Memory	Learning from historical data
Pattern Recognition	Detecting trends and anomalies
Decision-making	Predictive recommendations
Learning	Continuous model improvement

Multi-Layer Perceptron Regressor (MLPRegressor): It is a type of Artificial Neural Network (ANN) used in Machine Learning (ML) for solving regression problems, where the goal is to predict continuous numerical values rather than categories or classes.

1. Interpretation of the MLPRegressor Terminology

Term	Meaning
Multi-Layer	The network contains multiple layers of neurons
Perceptron	A basic artificial neuron or computational unit

Term	Meaning
Regressor	Used for predicting numerical values

2. Operation of MLPRegressor in Machine Learning

MLPRegressor learns relationships between:

- input variables,

  and

- numerical outputs.

It can model:

- linear relationships,
- nonlinear relationships,
- complex engineering behavior,
- and hidden patterns in data.

3. Examples of Regression Problems

In Chemical/Process Engineering

Predicting:

- reactor conversion,
- distillation column temperature,
- compressor efficiency,
- heat exchanger fouling resistance,
- pressure drop,
- product purity,
- refinery energy consumption,
- catalyst deactivation,
- emission levels,
- production rate.

These are continuous numerical outputs.

4. Structure of an MLPRegressor

An MLPRegressor consists of:

Layer	Function
Input Layer	Receives process data
Hidden Layers	Learn hidden relationships
Output Layer	Produces numerical prediction

5. Conceptual Architecture

Input Data → Hidden Layer(s) → Output Prediction

6. Example in Process Engineering

Suppose a refinery wants to predict:

- gasoline octane number.

Inputs:

- temperature,
- pressure,
- feed composition,
- reflux ratio,

- catalyst activity.

Output:

- predicted octane number.

The MLPRegressor learns from historical plant data.

Mass Balance: A first-principles equation based on conservation of mass. Mass entering, leaving, accumulating, being generated, or being consumed must be accounted for.

Mean Absolute Error (MAE): The average absolute difference between predicted and actual values.

Example: An MAE of 0.32 percentage point means that predicted purity differs from actual purity by approximately 0.32 percentage point on average.

Memory Cell: The internal component of an LSTM that preserves useful information over multiple time steps.

Methane Leakage: The unintended release of methane during natural-gas production, processing, transportation, storage, or use. Methane leakage can significantly affect the lifecycle carbon footprint of grey or blue hydrogen.

MLPRegressor: A Scikit-learn multilayer perceptron neural-network algorithm used for regression problems. It was applied in the presentation's distillation overhead-purity case study.

Model Parameters: Numerical values learned or adjusted by a model during training. In an ANN, the parameters include weights and biases.

Model Training: The process through which an ML or ANN model learns relationships from training data by adjusting its parameters.

Model Validation: The assessment of whether a model performs reliably on data that were not used to train it.

Monitoring: The continuous or periodic observation of process variables, equipment condition, alarms, and performance indicators.

Multivariate Data: Data containing several interacting variables measured at the same time. Refinery operations are highly multivariate because temperature, pressure, flow, composition, and equipment condition interact.

N

Natural Language Processing (NLP): is a field of Artificial Intelligence that enables computers to understand, interpret, summarize, generate, or respond to human language. NLP bridges the gap between human communication and machine intelligence, allowing AI systems to work with unstructured text, speech, and operator narratives.

Example: An engineer may ask, "Why did reactor conversion fall yesterday?" and an NLP system may summarize process trends and alarms.

1. The Importance of NLP in Engineering Applications

NLP mirrors the human brain's **language and communication** cognitive function:

- Understanding meaning
- Interpreting context
- Extracting insights
- Communicating information

This makes NLP essential for engineering environments where **reports, logs, procedures, and narratives** contain critical safety and operational knowledge.

2. NLP Applications in Chemical/Process Engineering

A. Incident and Safety Report Analysis

Plants generate thousands of text-based reports. NLP can:

- Extract root causes
- Identify recurring hazards
- Detect human-factor issues
- Summarize long narratives

Outcome: Better safety insights and proactive risk reduction

B. Alarm Log Interpretation

NLP analyzes alarm floods and operator comments to:

- Identify nuisance alarms
- Detect abnormal patterns
- Improve alarm rationalization

Outcome: More effective alarm management

C. Operator Logbook Analysis

Shift logs contain valuable experiential knowledge. NLP can:

- Detect trends in operator observations
- Highlight deviations
- Extract lessons learned

Outcome: Improved situational awareness

D. Procedure & SOP Optimization

NLP reviews Standard Operating Procedures to:

- Identify inconsistencies
- Flag ambiguous instructions
- Suggest improvements

Outcome: Clearer, safer procedures

E. Predictive Safety Analytics

NLP + ML models can forecast:

- Likely failure modes
- Human-error-related risks

- Process deviations

Outcome: Early warning and prevention

F. Knowledge Management

NLP powers intelligent search across:

- Technical manuals
- HAZOP reports
- Maintenance logs
- Engineering documents

Outcome: Faster access to critical knowledge

Nelson Complexity Index (NCI): A numerical measure used to compare the processing complexity and upgrading capability of petroleum refineries.

The index assigns a complexity factor to each process unit relative to the atmospheric crude distillation unit, which is assigned a factor of 1.0.

A simplified expression is:

$$\mathrm{NCI} = \sum_{i} \left(\frac{\text{Capacity of unit i}}{\text{Crude Distillation Capacity}} \right) \mathrm{x} \left(\text{Complexity Factor} \right)_{i} \quad (2)$$

A refinery with a high NCI generally contains more conversion, treating, upgrading, and product-improvement facilities than a simple refinery.

Example: A refinery containing FCC, hydrocracking, coking, catalytic reforming, alkylation, and extensive hydrotreating will generally have a higher NCI than a refinery consisting mainly of crude distillation and basic treating units.

A high NCI does not automatically indicate greater efficiency or profitability. It principally indicates greater processing complexity and potential upgrading capability.

Refinery Complexity

The following classification can be used to define the complexity of a refinery:

Simple refinery	It has atmospheric crude distillation, a catalytic reformer to produce high octane gasoline, and middle distillate hydrotreating units.
Complex refinery	It has in addition to the units of a simple refinery, conversion units such as hydrocrackers and fluid catalytic cracking units.

Ultra-complex refinery	The refinery has all of the units above in addition to deep conversion units, which convert atmospheric or vacuum residue into light products.

The complexity of a refinery can be assessed by calculating the complexity factor. Each unit has a coefficient of complexity (CC_i) defined as the ratio of the capital cost of the unit per ton of feedstock to the capital cost of the crude distillation unit (CDU) per ton of feedstock. The complexity factor (Cf_i) of the whole refinery is then calculated from the coefficients of complexity for the units in the refinery as follows:

$$CF = \sum_{i}^{N} \left(\frac{F_i}{F_{CDU}} \right) CC_i \qquad (3)$$

where F_i and F_{CDU} are the feed rate to unit i and CDU respectively.

Example

Calculate the complexity factor for a refinery which has the following unit data.

Unit	**Complexity coefficient (CC_i)**	**Percent capacity relative to CDU capacity (F_i/F_{CDU})**

Vacuum distillation unit	1.5	40
Fluid catalytic cracking	7	25
Hydrocracking	7	15
Hydrotreating	5	50
Reforming	3.4	30
Alkylation	6	5

Solution

From Eq. 3

CF = 0.40 x 1.5 + 0.25 x 7 + 0.15 x 7 + 0.50 x 5 + 0.3 x 3.4 + 0.05 x 6 = 7.8

The following terms are part of the refinery margins:

Hydrocarbon Margin (HCM)	The difference between the aggregate value of the products and the aggregate value of the crudes and feedstocks required for the refining.

	It is not the true measure of the refinery's profit, but it can only give a good approximation of the refinery's profitability for a particular configuration. It is used to approximate the profitability if a change in refinery configuration or operating modes and conditions are being considered. It is used to calculate the "Gross Refinery Margin" or GRM.
Gross Refinery Margin (GRM)	Is the refinery's margin after deducting all variable cost from the Hydrocarbon Margin. It is the preferred parameter for indicating the refining profitability as it includes all variable cost incurred during the refining process.
Variable Cost	This varies with throughput of the refinery such as imported feedstock, chemicals, catalyst, maintenance, utilities and purchased energy (e.g., natural gas and electricity).
Net Refinery Margin	
Fixed cost	This does not vary with refinery throughput. The fixed costs in the short term are manpower,

maintenance, insurance, administration and depreciation.

Stream that can be readily valued are namely:

- Ready products, crude oil and imported feedstocks.
- Blending components
- Intermediate feedstocks.

Ready products, crude oil and other feedstocks are normally valued at market price. If we consider the following:

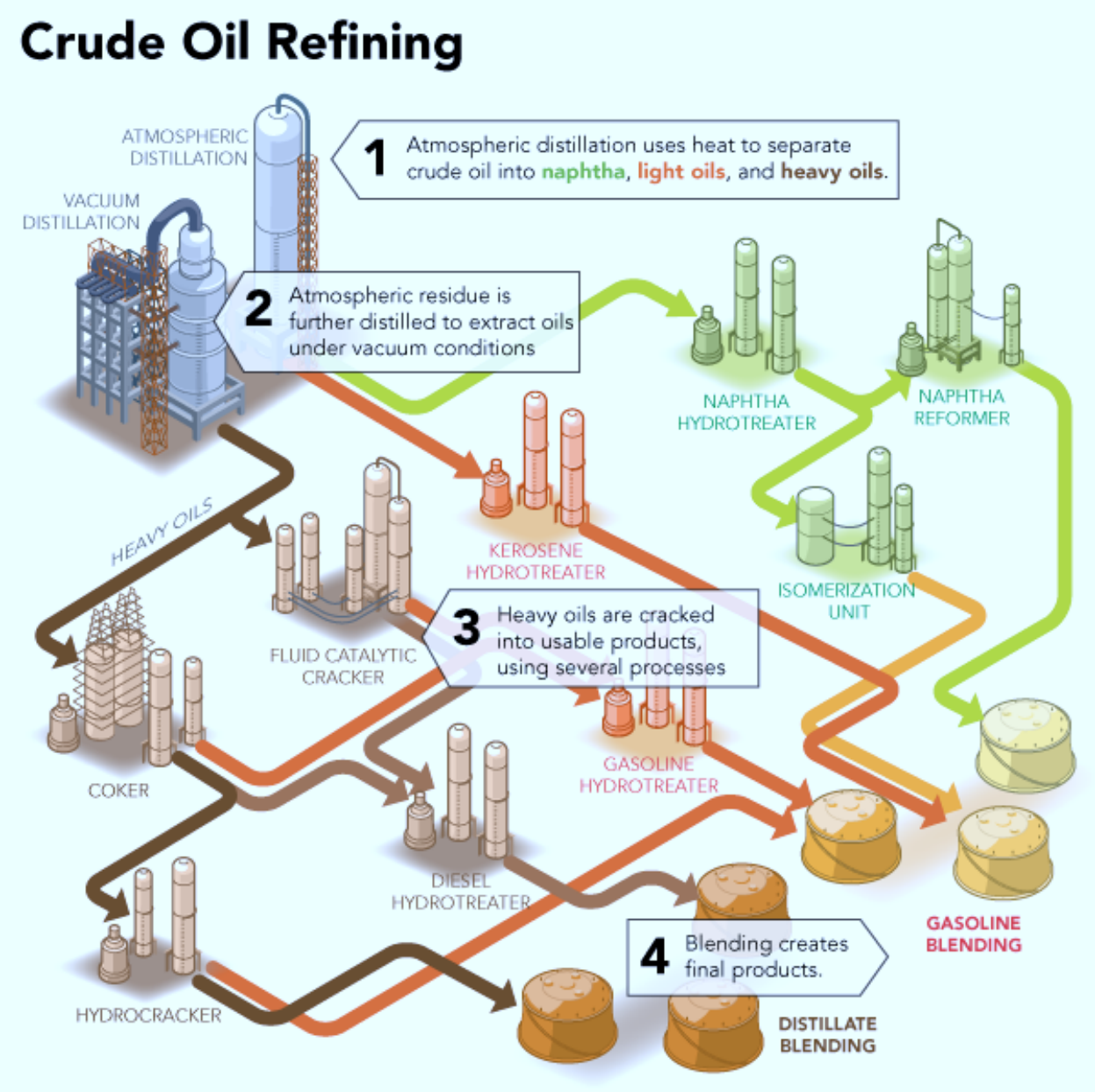


Figure 25. Petroleum crude oil refining processes.

Neural Networks: Is a computational model inspired by the structure and functioning of the human brain. It consists of interconnected "neurons" or nodes that process information and learn patterns from data.

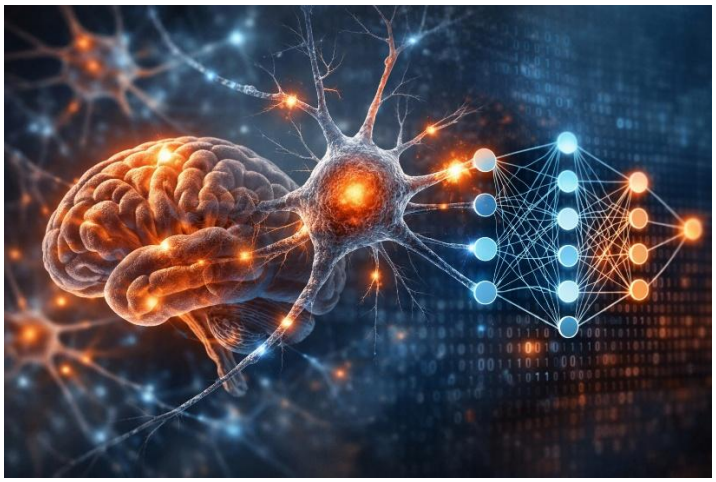


Figure 26. A combine composite of the human brain + neurons + Artificial Neural Network Systems (ANNS) (Source: Author's illustrative visualization developed with AI-assisted tools.)

Figure 26 shows the combined composite image of the human brain + biological neuron + artificial neural network (ANN)

This composite visual shows:

- The human brain as the biological inspiration.
- A biological neuron with dendrites, axon, and synapses.
- An artificial neural network with interconnected nodes that mimic information flow.

Neural networks are a major component of AI and ML systems.

They are particularly useful for:

- pattern recognition,
- prediction,
- classification,
- optimization,
- anomaly detection, and
- nonlinear process modeling.

Neuron: A specialized biological cell that receives, processes, and transmits information. Artificial neural networks are loosely inspired by neuronal connectivity (See Figures 18f, 22).

Neuron Cell: Another expression for a biological neuron. Its principal components include dendrites, the soma or cell body, the axon, and synapses.

Neurotransmitter: A chemical messenger released at a biological synapse to transmit a signal from one neuron to another.

Nonlinear Relationship: A relationship in which the output does not change in direct proportion to the input. Many refinery and chemical-process relationships are nonlinear.

Normal Operating Envelope: The range of process conditions within which a plant or equipment item is expected to operate safely and satisfactorily.

O

Optimization: The process of identifying the best operating or design conditions subject to technical, economic, safety, and environmental constraints.

Optimization Algorithms: are mathematical and computational methods used to **find the best possible solution** to a problem under a set of constraints. They work by systematically adjusting variables to:

- Minimize cost
- Maximize efficiency
- Improve performance
- Satisfy safety and operational limits

In engineering, optimization algorithms help determine **optimal operating conditions**, **resource allocation**, **control strategies**, and **design parameters**.

1. The importance of Optimization Algorithms

Optimization algorithms mirror human cognitive functions:

- **Perception** → understanding system inputs
- **Memory** → storing past solutions
- **Decision-making** → selecting the best option
- **Learning** → improving over iterations

They are the computational counterpart to **engineering judgment**.

2. Types of Optimization Algorithms

Each includes a Guided Link for deeper exploration.

A. Linear Programming (LP): Used when relationships are linear. Applications: blending, resource allocation, scheduling.

B. Nonlinear Programming (NLP): Handles nonlinear equations common in chemical processes. Applications: reactor optimization, distillation energy minimization.

C. Mixed-Integer Programming (MIP): Combines continuous and discrete decisions. Applications: batch scheduling, equipment selection.

D. Genetic Algorithms (GA): Evolution-inspired search for global optima. Applications: heat exchanger network design, catalyst optimization.

E. Gradient-Based Methods: Use derivatives to find optimal points quickly. Applications: MPC tuning, process parameter optimization.

F. Heuristic and Metaheuristic Methods: Rule-based or probabilistic search. Applications: plant layout, supply chain optimization.

G. Reinforcement Learning (RL): AI learns optimal actions through trial and reward. Applications: autonomous control, adaptive optimization.

3. Optimization Algorithms in Chemical/Process Engineering

A. Distillation Column Optimization

- Minimize reboiler duty
- Maximize product purity
- Optimize reflux ratio

Outcome: Lower energy use and improved separation

B. Reactor Optimization

- Maximize conversion or selectivity
- Optimize temperature and feed ratios
- Manage exothermic behaviour

Outcome: Higher yield and safer operation

C. Heat Exchanger Network Optimization

- Minimize utility consumption
- Optimize heat recovery

Outcome: Reduced operating cost

D. Plant-Wide Optimization

- Integrate multiple units
- Balance steam, cooling water, and utilities

Outcome: Holistic efficiency improvements

E. Supply Chain and Scheduling

- Optimize batch sequences

- Minimize inventory and downtime

Outcome: **Higher throughput and reliability**

4. Optimization Algorithms + AI/ML

Optimization and AI/ML are complementary:

Optimization Role	AI/ML Enhancement	Engineering Benefit
Objective function	ML predicts outcomes	More accurate optimization
Constraints	AI detects limits dynamically	Safer operations
Search strategy	RL explores new solutions	Adaptive optimization
Parameter tuning	ML automates tuning	Faster convergence
Scenario analysis	Digital twins simulate outcomes	Better decisions

Together, they enable **self-optimizing plants** in Industry 4.0.

5. Cognitive Functions Connection

Cognitive Function	Optimization Role
Decision-making	Choosing best operating conditions
Learning	Iterative improvement of solutions
Memory	Using historical performance data
Perception	Interpreting process constraints
Communication	Explaining trade-offs and results

Output Gate: The LSTM component that determines which information from the memory cell should be passed to the next stage.

Output Layer: The final ANN layer that produces the prediction, classification, or calculated result.

Overhead Purity: The concentration or percentage of the required light component in the overhead product from a distillation column.

Operational Feedback: Information from the physical process that is returned to a model or digital twin to update predictions and improve performance.

P

Partial Least-Squares Regression (PLS): A regression method useful when input variables are numerous and strongly correlated. It is commonly applied to product-quality soft sensors.

Pattern Recognition: The identification of recurring relationships, structures, trends, or signatures within data.

Perception: The cognitive ability to recognize and interpret information received through the senses or instrumentation.

Physics-Based Model: A model constructed using established physical and chemical laws. It is closely related to a first-principles model.

Physics-Informed AI: An AI approach in which physical laws, engineering constraints, or first-principles relationships are incorporated into model development.

PI Historian: An industrial time-series data system used to collect, store, organize, retrieve, and analyse historical and real-time plant operating data.

The term commonly refers to the historian functions provided through the **AVEVA PI System**, formerly associated with OSIsoft. At the centre of the system is a time-series data archive that stores process measurements collected from instrumentation, control systems, equipment-monitoring systems, and other industrial data sources.

A PI Historian may receive information from:

- Distributed Control Systems
- Supervisory Control and Data Acquisition systems
- Programmable Logic Controllers
- Laboratory systems
- Equipment-condition-monitoring systems
- Smart sensors
- Process analysers
- Utility-management systems

Typical applications include:

- Process-trend analysis

- Production-performance monitoring
- Energy analysis
- Equipment-health monitoring
- Process troubleshooting
- Predictive maintenance
- Fault and anomaly detection
- AI and machine-learning model training
- Digital-twin development
- Process-safety investigations

Example: A refinery may store reactor temperature, pressure, feed rate, cooling-water flow, catalyst activity, and product composition in a PI Historian. Engineers can retrieve these data to determine why reactor conversion decreased or why temperature increased unexpectedly.

Prediction: The estimation of a future or unknown process value using a model.

Example: Predicting the future fouling rate of a heat exchanger.

Predictive Analytics: a. Is about using data, statistical models, and machine-learning techniques to anticipate what is likely to happen next. **b**.

Predictive Analysis (or Predictive Analytics) is the use of historical data, statistical methods, Artificial Intelligence (AI), Machine Learning (ML), and mathematical models to predict future events, trends, behaviors, or process outcomes. It involves analyzing past and present operating conditions to estimate what is likely to occur in the future.

Predictive analysis helps engineers and organizations make proactive decisions rather than simply reacting to problems after they occur. By identifying patterns and relationships within large datasets, predictive models can forecast equipment performance, process behavior, safety risks, product quality, and operational efficiency.

In simple terms, predictive analysis answers the question:

“What is likely to happen next based on available data and learned patterns?”

Relationship Between Predictive Analysis and AI/ML

Predictive analysis often uses:

- Historical process data
- Artificial Neural Networks (ANN)
- Machine Learning algorithms
- Statistical regression models

- Pattern recognition techniques
- Real-time monitoring systems

AI and ML improve predictive analysis by enabling systems to continuously learn from new operating data and improve prediction accuracy over time.

Predictive Maintenance (PdM): Is a maintenance strategy that uses real-time operating data, historical equipment information, sensors, AI, ML, and predictive analysis techniques to determine when equipment is likely to fail or require maintenance before an actual breakdown occurs.

Unlike traditional maintenance approaches, predictive maintenance continuously monitors equipment condition and predicts future problems based on operational patterns, trends, and abnormal behavior.

In simple terms, predictive maintenance answers the question:

“When is the equipment likely to fail, and what action should be taken before failure occurs?”

Principle of Predictive Maintenance

Predictive maintenance works by collecting and analyzing data such as:

- Temperature
- Pressure

- Vibration
- Flow rate
- Noise
- Power consumption
- Corrosion rate
- Equipment efficiency
- Lubrication condition

AI and ML algorithms analyze these operating conditions to identify early warning signs of deterioration, wear, fouling, corrosion, overheating, vibration problems, or process instability.

Process Historian: A specialized industrial database designed to store large quantities of time-stamped process, alarm, event, and equipment data.

Unlike a conventional business database, a process historian is designed for rapidly changing operational measurements collected continuously from industrial facilities.

Example: A process historian may store one reactor-temperature value every second for several years, allowing engineers to examine operating trends before and after an incident.

Principal Component Analysis (PCA): A statistical method that reduces many correlated measurements into a smaller number of principal components representing the dominant patterns in the data.

Probabilistic Model: A model that represents uncertainty and may provide a likely value, range, probability, or confidence interval rather than one fixed result.

Process Intelligence: The conversion of process data into useful operating knowledge through contextualization, analytics, visualization, modelling, prediction, and decision support.

Process Intelligence Platform: An integrated digital environment that collects, organizes, contextualizes, analyses, and presents industrial-process information to support monitoring, diagnosis, prediction, optimization, and decision-making.

A Process Intelligence Platform may integrate information from:

- Distributed Control Systems

- Supervisory Control and Data Acquisition systems
- Plant historians
- Laboratory information-management systems
- Maintenance-management systems
- Equipment-condition-monitoring systems
- Process simulators
- Digital twins
- AI and machine-learning models
- Production and business systems

Example: A refinery Process Intelligence Platform may combine crude-unit temperatures, pressures, flow rates, laboratory results, furnace efficiency, exchanger fouling, maintenance records, and AI predictions within one operating environment.

A Process Intelligence Platform is broader than an individual AI model. The platform provides the connected data and operating environment, while AI/ML models provide specific predictive or analytical functions.

Process Optimization: The adjustment of operating conditions to improve production, quality, energy use, emissions, safety, reliability, or profitability.

Process Safety Management (PSM): A systematic framework for managing hazards associated with highly hazardous processes through engineering, operating, maintenance, training, and management practices.

Process Safety Monitoring: Is the continuous observation, measurement, analysis, and evaluation of process operating conditions, equipment performance, and safety-related parameters to detect abnormal situations, prevent hazardous events, and maintain safe operation within a chemical or process plant.

It involves the use of sensors, instrumentation, alarms, control systems, AI, ML, and real-time data analysis to identify unsafe operating conditions before they escalate into accidents, equipment failures, fires, explosions, toxic releases, or environmental incidents.

In simple terms, process safety monitoring answers the question:

“Is the process operating safely, and are there early signs of danger or abnormal conditions?”

Process Simulation: The computational representation of a chemical, petroleum, energy, or manufacturing process using mathematical equations, thermodynamic models, equipment models, reaction kinetics, and engineering correlations.

Process simulation may be used to calculate:

- Material balances
- Energy balances
- Phase equilibria
- Equipment duties
- Product compositions
- Utility requirements
- Pressure losses
- Process responses
- Economic performance

Common process-simulation packages include Aspen HYSYS, Aspen Plus, Honeywell UniSim Design, CHEMCAD, and PRO/II.

Example: A crude-distillation-unit simulation may calculate product yields, tray temperatures, condenser duty, furnace duty, pumparound performance, and product properties.

Process Simulation and AI Integration: The combination of deterministic process simulation with AI or machine learning.

The simulator provides physically based calculations, while the AI model may provide:

- Rapid surrogate predictions
- Plant-data corrections
- Fouling estimates
- Fault detection
- Real-time optimization
- Uncertainty assessment

Example: A process simulator predicts the theoretical outlet temperature of a heat exchanger, while an ML model corrects the result using actual plant-fouling data.

Product-Quality Soft Sensor: A model that estimates a product property from readily available process measurements.

Example: Predicting sulfur concentration from temperature, pressure, flow, and composition data.

Python: A widely used programming language for engineering calculations, numerical analysis, data processing, process simulation, data analysis, visualization, automation, artificial intelligence, and machine learning and AI model development.

In chemical and process engineering, Python may be used for:

- Mass- and energy-balance calculations
- Reactor modelling
- Distillation prediction
- Process-data cleaning
- PI historical-data analysis
- Plotting process trends
- Fault and anomaly detection
- Machine-learning model development
- Digital-twin calculations
- Process optimization

Brief Python Example: Analysing Process-Historian Data

The following example represents reactor-temperature data that could have been exported from a PI Historian. The script calculates a rolling average and identifies measurements above a high-high-temperature limit.

```
import pandas as pd


# Example reactor-temperature history
```

```
data = {
    "Time": pd.date_range(
        start="2026-08-05 08:00",
        periods=8,
        freq="5min"
    ),
    "Reactor_Temperature_C": [
        150.0, 151.2, 152.5, 155.0,
        160.8, 168.5, 181.0, 188.0
    ]
}

history = pd.DataFrame(data)

# Calculate a three-reading rolling average
history["Rolling_Average_C"] = (
    history["Reactor_Temperature_C"]
    .rolling(window=3, min_periods=1)
    .mean()
)

# Define the high-high temperature limit
```

```
high_high_limit = 180.0


# Identify potentially unsafe readings
history["High_High_Alarm"] = (
    history["Reactor_Temperature_C"] >= high_high_limit
)


print(history)
```

Engineering Interpretation

The script performs four basic functions:

1. Creates or receives time-stamped process data.
2. Calculates the recent average reactor temperature.
3. Compares each measurement with a defined safety limit.
4. Flags measurements at or above 180°C.

The final two readings would be marked True under High_High_Alarm, indicating that the reactor temperature has reached or exceeded the defined limit.

In an operational application, the data would normally be retrieved from an authorized historian interface rather than manually entered. The result could

support engineering investigation, early-warning analysis, or operator decision support. It would not, by itself, replace an independently designed and validated Safety Instrumented Function.

Python Script: A file or sequence of Python instructions written to perform a calculation, data-processing task, simulation, visualization, or automation function.

Python scripts normally use the .py file extension.

Example: A script named:

jacketed_cstr_cooling_failure.py

may calculate reactor concentration and temperature under normal-cooling and cooling-failure conditions.

Another script named:

distillation_overhead_purity_ann.py

may train an artificial neural network to predict overhead purity from refinery operating variables.

Python Library: A collection of prewritten functions and tools that can be imported into a Python program.

Common engineering and AI libraries include:

- **NumPy** — numerical calculations and arrays
- **Pandas** — data tables and time-series analysis
- **Matplotlib** — plots and engineering graphs
- **SciPy** — scientific calculations and differential equations
- **Scikit-learn** — machine-learning models and evaluation
- **TensorFlow** — neural networks and deep learning
- **PyTorch** — neural networks and deep-learning research

Example:

```
import pandas as pd
import matplotlib.pyplot as plt
```

These instructions import Pandas for process-data analysis and Matplotlib for plotting process trends.

Example: In a chemical plant, Python code may read temperature, pressure, and flow-rate data from a reactor. An ML model can then learn from past operating data and predict whether the reactor is operating safely or moving toward an abnormal condition.

This helps engineers take corrective action before problems become serious.

Engineering Importance: Python connects engineering knowledge with AI/ML tools. It allows chemical and process engineers to transform plant data into useful predictions, plots, warnings, and decisions. Therefore, Python is not only a programming language; it is also a practical tool for modern process simulation, troubleshooting, optimization, and safety improvement.

Q

Quality Prediction: The estimation of a product property using process measurements and a predictive model.

Example: Predicting gasoline octane number or distillation overhead purity.

Quality Soft Sensor: A data-driven model that continuously estimates product quality when direct laboratory measurements are delayed, costly, or unavailable.

Quantitative Risk Assessment (QRA): A numerical assessment of the frequencies and consequences of hazardous events, used to estimate individual, societal, or facility risk.

R

Random Forest: A machine-learning method that combines many decision trees to produce a prediction or classification.

Real-Time Optimization (RTO): Is an advanced process control and decision-making system that continuously monitors plant operating conditions and automatically adjusts process variables to achieve the best possible operational performance in real time.

RTO combines:

- Process measurements
- Mathematical models
- Artificial Intelligence (AI)
- Machine Learning (ML)
- Optimization algorithms
- Real-time plant data

to determine the most economical, efficient, safe, and reliable operating conditions for a chemical or process plant.

In simple terms:

Real-Time Optimization continuously asks: “What are the best operating conditions for the plant right now?”

Principle of Real-Time Optimization

RTO systems collect real-time process data such as:

- Temperature
- Pressure
- Flow rate
- Composition
- Energy consumption
- Equipment performance
- Product quality

The system then compares actual plant performance with desired operating targets and automatically recommends or adjusts operating parameters to optimize performance.

Reasoning: The ability to analyse information logically, evaluate evidence, and reach sound conclusions.

Recurrent Neural Network (RNN): A neural-network architecture designed for sequential data. It passes information from one time step to the next but may have difficulty retaining long-term dependencies.

Regression: A statistical or machine-learning method used to predict a continuous numerical value.

Reinforcement Learning: A machine-learning approach in which an agent learns actions through rewards and penalties. It may be used to investigate process-control or optimization strategies.

Remaining Useful Life (RUL): The predicted time remaining before equipment fails or reaches an unacceptable performance limit.

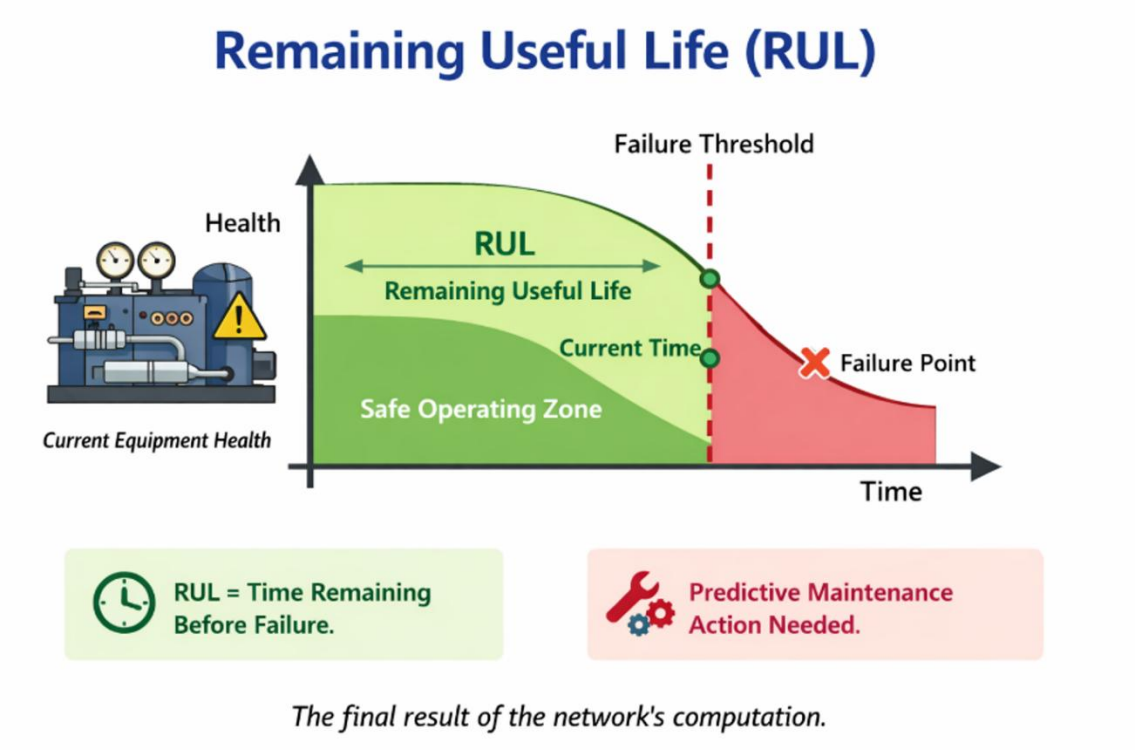


Figure 27. Remaining Useful Life (RUL)

RUL stands for Remaining Useful Life. In engineering, maintenance, and reliability modelling, Remaining Useful Life refers to: How much time is left before a component, machine, or system fails or reaches an unacceptable performance threshold. It is a prediction made using sensor data, historical failures, and AI/ML models (including LSTMs). It is central to predictive maintenance, where the goal is to anticipate failure before it happens so that maintenance can be scheduled optimally.

Figure 27 illustrates how Remaining Useful Life (RUL) represents the time interval between the current condition of equipment and its predicted failure point. It shows a health-versus-time curve, where the system's performance

gradually declines toward a failure threshold. The green section indicates the safe operating zone, while the red section marks the failure zone. The arrow labelled RUL highlights the remaining time before failure, emphasizing how predictive maintenance can be scheduled proactively to prevent downtime.

Residual: The difference between an observed value and the value predicted or reconstructed by a model. Large residuals may indicate an abnormal condition.

Ridge Regression: A regression method that applies a penalty to model coefficients to reduce overfitting and improve stability.

Risk-Reduction Factor (RRF): A numerical expression of how much a safeguard or Safety Instrumented Function reduces risk.

Robotics: is the field of engineering and computer science that focuses on the design, construction, operation, and intelligent control of robots, machines capable of performing tasks autonomously or semi-autonomously.

Robotics integrates:

- Mechanical engineering
- Electrical/electronic engineering
- Computer science

- AI/ML
- Control systems

In modern industry, robots extend human capability by performing tasks that are **dangerous, repetitive, precise, or require high endurance**.

Types of Robots in Industry

Each type includes a Guided Link for deeper exploration.

- **Industrial Robots** — articulated arms for welding, assembly, packaging
- **Mobile Robots** — AGVs, AMRs for material handling
- **Collaborative Robots (Cobots)** — robots designed to work safely alongside humans
- **Inspection Robots** — drones, crawlers for inspection of hazardous areas
- **Service Robots** — cleaning, monitoring, logistics
- **Autonomous Robots** — robots that make decisions using AI/ML

Robotics in Chemical/Process Engineering

Robotics is increasingly used in process industries to improve safety, reliability, and efficiency.

Root Mean Squared Error (RMSE): A model-error measure that gives greater emphasis to larger prediction errors.

Example: An RMSE of 0.39 percentage point indicates that the typical overhead-purity prediction error is approximately 0.39 percentage point, with additional weighting applied to larger deviations.

Runaway Reaction: A rapidly accelerating reaction in which heat generation exceeds heat removal, causing temperature and reaction rate to rise uncontrollably.

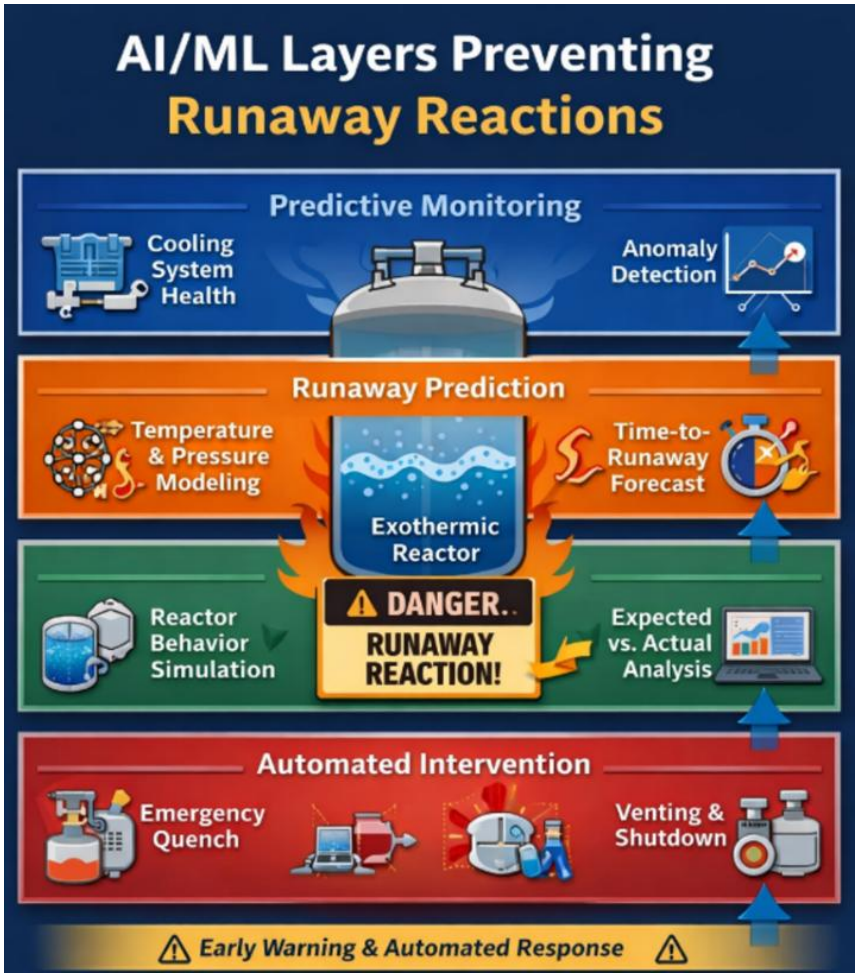


Figure 28. AI/ML layers in preventing runaways

R^2, Coefficient of Determination: A statistical measure of the proportion of variation in the output explained by a model.

Example: An R^2 of 0.9324 means that the ANN explains approximately 93.24% of the variation in overhead purity.

S

Safe Operating Limits (SOLs): Defined operating boundaries within which a process must remain to prevent unsafe conditions or equipment damage.

Safety Instrumented Function (SIF): A specific protective function designed to place a process into a safe condition when predetermined hazardous conditions are detected.

A Safety Instrumented Function normally consists of:

- Sensors
- A logic solver
- Final control elements

Example: A high-high reactor-temperature sensor may send a signal to a logic solver, which closes the reactant-feed valve and initiates emergency cooling.

Safety Instrumented Level: A phrase sometimes used informally when referring to the required reliability of a safety instrumented protective function. The established functional-safety term is **Safety Integrity Level**.

Safety Instrumented System (SIS): An independent system composed of sensors, logic solvers, and final control elements that performs one or more Safety Instrumented Functions.

Safety Integrity Level (SIL): A discrete performance classification indicating the required risk-reduction capability or reliability of a Safety Instrumented Function.

The four levels are:

- SIL 1
- SIL 2
- SIL 3
- SIL 4

For low-demand operation, increasing SIL corresponds to increasing required risk reduction:

Safety Integrity Level	Approximate Risk-Reduction Factor
SIL 1	10 to 100
SIL 2	100 to 1,000
SIL 3	1,000 to 10,000
SIL 4	10,000 to 100,000

SIL applies to a specific Safety Instrumented Function, not automatically to an entire plant, control system, instrument, or item of equipment.

Example: A reactor high-high-temperature shutdown may be assigned SIL 2 after hazard analysis and LOPA determine that a risk-reduction factor between 100 and 1,000 is required.

AI may support diagnostics, testing, condition monitoring, and maintenance of safety-related equipment, but an unverified AI model should not automatically be treated as a credited SIL protection layer.

Scikit-Learn: A Python machine-learning library containing algorithms for regression, classification, preprocessing, neural networks, and model evaluation.

Self-Supervised Learning: A learning approach in which useful training signals are derived from the data itself rather than being supplied entirely through manually labelled examples.

Sensor Drift: A gradual change in sensor output that causes the measurement to become inaccurate over time.

Sensor Noise: Random fluctuations or disturbances in measured signals that do not represent actual process changes.

Signal Interpretation: The analysis of measurements such as vibration, pressure, temperature, flow, images, or acoustic data to determine process or equipment condition.

Simulation: The use of a mathematical or computational model to reproduce the behaviour of a process or system.

Soft Sensor: A mathematical or data-driven model that estimates a variable that is difficult, expensive, or slow to measure directly.

Soma: The cell body of a biological neuron. It receives and processes signals collected through the dendrites.

Sour Crude Oil: Crude oil containing a comparatively high concentration of sulfur compounds, including hydrogen sulfide and organic sulfur compounds.

A commonly used industry distinction describes crude oil containing more than approximately 0.5 weight percent sulfur as sour, although commercial definitions may vary.

Sour crude generally requires more extensive:

- Desalting
- Hydrotreating

- Sulfur removal
- Corrosion control
- Hydrogen consumption
- Sulfur-recovery capacity

Example: A high-sulfur heavy crude may require severe hydrotreating and substantial hydrogen consumption before its products satisfy low-sulfur fuel specifications.

Steady-State Process Simulation: A simulation in which process variables are assumed not to change with time. Accumulation terms are normally taken as zero.

Support Vector Machine (SVM): A machine-learning algorithm used primarily for classification and, in adapted form, regression.

Support Vector Regression (SVR): The regression form of a support vector machine. It may be used as a surrogate model for process prediction.

Surrogate Model: A simplified mathematical or data-driven approximation of a more complex process or model. It provides rapid predictions without repeatedly solving the complete first-principles equations.

Example: An ANN may act as a surrogate for a CSTR by mapping feed conditions and residence time to conversion and outlet concentration.

Sweet Crude Oil: Crude oil containing a comparatively low concentration of sulfur compounds.

A commonly used industry distinction describes crude oil containing less than approximately 0.5 weight percent sulfur as sweet, although commercial specifications may vary.

Sweet crude generally requires less sulfur removal than sour crude.

Example: A light sweet crude with high API gravity and low sulfur content may yield significant quantities of naphtha, kerosene, and diesel with comparatively lower treating requirements.

The terms **sweet** and **sour** describe sulfur content, whereas **light** and **heavy** principally describe density or API gravity.

Synapse: The junction through which one biological neuron communicates with another. In an ANN analogy, a synapse corresponds to a weighted connection.

Synaptic Plasticity: The ability of biological synapses to strengthen or weaken through experience, forming a basis for biological learning and memory.

Supervisory Control and Data Acquisition (SCADA) systems: A SCADA system is an industrial automation and monitoring architecture used to collect real-time data, supervise remote equipment, and control distributed assets across large-scale operations.

SCADA is essential for industries where equipment is spread across wide geographic areas as pipelines, tank farms, utilities, offshore platforms, and remote production sites.

It provides:

- Centralized monitoring
- Remote control
- Data acquisition
- Alarm management
- Historical trending
- Operator visualization

SCADA is the **eyes and ears** of geographically distributed process operations.

T

Teamwork: a. is the ability of diverse individuals to work together toward a shared goal with clarity, trust, and coordinated effort. In today's engineering world—where AI, digital tools, and complex systems shape daily operations—teamwork is not just helpful; it is **mission-critical**. **b**. is the collaborative effort of individuals working together toward a common goal by sharing knowledge, skills, responsibilities, ideas, and resources to achieve successful outcomes efficiently and safely.

In engineering, teamwork involves professionals from different disciplines cooperating to solve technical, operational, safety, economic, and organizational problems. Effective teamwork requires:

- Communication
- Cooperation
- Trust
- Coordination
- Leadership

- Mutual respect
- Shared responsibility
- Problem-solving ability

In simple terms: **Teamwork means combining the strengths, knowledge, and experience of different people to achieve a common engineering objective.**

Importance of Teamwork in Engineering

Engineering projects are often highly complex and multidisciplinary. No single engineer possesses all the expertise needed to design, operate, maintain, and optimize large industrial systems. Teamwork therefore becomes essential for successful engineering practice.

Teamwork in Petroleum and Petrochemical Industries

The petroleum and petrochemical industries are among the most multidisciplinary engineering sectors in the world. Large facilities such as:

- Refineries
- Petrochemical plants
- LNG plants
- Offshore platforms

- Pipelines
- Gas processing facilities

require collaboration among many specialists.

Temperature Runaway: A rapid and uncontrolled rise in reactor temperature caused by excessive heat generation and insufficient heat removal.

Thermodynamics: The branch of engineering science concerned with energy, heat, work, equilibrium, and the properties of matter.

Time-Series Data: Measurements recorded in chronological order.

Example: Reactor temperature recorded every second or compressor vibration recorded every minute.

Training Data: Historical, laboratory, simulated, or real-time examples used to teach an ML model.

Transformer: A deep-learning architecture capable of learning long-range relationships within sequences. Transformers support modern generative AI, language processing, code generation, and multivariate forecasting.

Tray Efficiency: A measure of how closely an actual distillation tray approaches ideal equilibrium-stage performance.

Troubleshooting: The structured identification and correction of the causes of process or equipment problems.

U

UA Heat-Transfer Parameter: The product of the overall heat-transfer coefficient, U, and heat-transfer area, A. It represents the heat-transfer capability of equipment such as a reactor jacket or heat exchanger.

Example: In the CSTR cooling-failure case, setting UA to zero represents complete loss of cooling.

Uncertainty: The variability or lack of exact knowledge caused by sensor noise, changing feed composition, catalyst ageing, fouling, weather effects, human operation, or unknown disturbances.

UniSim Design: A deterministic process-simulation package used to model chemical and petroleum processes using first-principles relationships.

Unsupervised Learning: A machine-learning approach that identifies patterns, groupings, structures, or anomalies in data without requiring predefined output labels.

V

Validation Dataset: Data used to assess model performance and support model selection without being used directly to fit the final model parameters.

Variational Autoencoders (VAEs): is a type of **generative model** that learns how to represent complex data (images, signals, spectra, molecular structures, etc.) in a **compressed latent space**, and then uses that space to **generate new data** with similar characteristics. It is inspired by the **probabilistic structure of the human brain**, where information is encoded, compressed, and reconstructed through neural pathways.

Process Engineering Analogy for the Operation of a Variational Autoencoder (VAE)

Component	Function	Analogy
Encoder	Compresses input data into a latent vector (mean + variance)	Like reducing a full PFD into key design parameters

Component	Function	Analogy
Latent Space	A learned probability distribution of the data	Like a design space of feasible operating conditions
Decoder	Reconstructs or generates new data from latent vectors	Like generating new process configurations from design parameters

VAEs do not memorize data — they **learn the underlying distribution**, allowing them to generate **new, realistic variations**.

Importance of VAEs in Generative AI

VAEs are one of the foundational models in **Generative AI** because they can:

- Create **new samples** similar to the training data
- Interpolate smoothly between data points
- Learn **continuous latent representations**
- Generate **probabilistic outputs** (useful for uncertainty quantification)
- Work well with **limited or noisy datasets**

They are widely used in image generation, molecular design, anomaly detection, and simulation.

Applications of VAEs in Chemical & Process Engineering

VAEs are extremely powerful for engineering because they can model **complex, nonlinear, high-dimensional systems** exactly the kind found in chemical processes.

The following are the most relevant applications:

1. Reaction Mechanism Generation

VAEs can generate **new reaction pathways**, estimate missing kinetic parameters, or propose alternative mechanisms.

Useful for:

- Catalyst development
- Combustion modeling
- Polymerization kinetics

2. Process Simulation and Surrogate Modeling

VAEs can learn the behaviour of complex unit operations and create **fast surrogate models**.

Examples:

- Distillation column behaviour

- Reactor conversion profiles
- Heat exchanger performance

3. Fault Detection and Anomaly Identification

VAEs learn the “normal” operating distribution. Anything outside that distribution is flagged as abnormal.

Applications:

- Early detection of pump failure
- Identifying off-spec product
- Detecting runaway reaction signatures

4. Process Optimization and Design Space Exploration

VAEs can generate **new feasible operating points** or **new process configurations**.

Examples:

- Generating alternative PFDs
- Exploring optimal reactor conditions
- Designing energy-efficient heat-integration networks

5. Molecular and Catalyst Design

VAEs can generate new molecules or catalyst structures with desired properties.

Applications:

- Zeolite design
- Metal–organic frameworks
- Polymer precursors

Vapor-Liquid Equilibrium (VLE): The thermodynamic relationship between vapor and liquid compositions at equilibrium. VLE is fundamental to distillation design and simulation.

Vibration Analysis: The examination of machinery-vibration signals to identify problems such as imbalance, misalignment, cavitation, bearing wear, or compressor instability.

Virtual Representation: A computerized representation of a physical process, asset, or system. A digital twin is an operationally connected and continuously updated virtual representation.

W

Waste Minimization: The reduction of material losses, off-specification products, emissions, and unnecessary resource consumption through improved design and operation.

Weight: A numerical parameter assigned to a connection between artificial neurons. The weight indicates the influence of one input or neuron on another.

Weight Optimization: The adjustment of ANN weights during training to reduce the difference between predicted and actual outputs.

White Hydrogen: Naturally occurring hydrogen produced by geological or geochemical processes and found in underground formations.

It is also called:

- Natural hydrogen
- Geological hydrogen
- Native hydrogen
- Geologic hydrogen

Potential processing stages may include:

- Well production
- Gas-liquid separation
- Moisture removal
- Compression
- Carbon dioxide removal
- Hydrogen sulfide removal
- Dehydration
- Membrane separation
- Pressure swing adsorption
- Product compression and export

Example: A geological gas stream containing hydrogen, nitrogen, methane, water, carbon dioxide, or hydrogen sulfide may require extensive purification before industrial use.

Wisdom: The human ability to combine knowledge, experience, ethics, context, empathy, and judgment when deciding how information should be used.

X

X-Axis: The horizontal axis of a graph, normally used to represent an independent variable or time.

Example: In a reactor cooling-failure plot, the x-axis may represent elapsed operating time.

X Variables: A general mathematical notation for model inputs or independent variables.

Example: In the distillation-purity model, the X variables include feed temperature, reflux ratio, feed composition, pressure, and tray efficiency.

Y

Yield: The quantity of desired product obtained relative to the feed or reactant supplied.

Yield Estimation: The use of engineering models or AI to predict the quantity of a desired product.

Example: Predicting gasoline and LPG yields from an FCC unit.

Yield Optimization: The identification of operating conditions that maximize production of desired products while satisfying product-quality, safety, equipment, energy, and environmental constraints.

Z

Zero-Carbon Energy: Energy generated with no direct carbon dioxide emissions during operation. Renewable electricity used for green-hydrogen manufacture is an example.

Zero-Cooling Condition: A modeled condition in which the reactor's heat-removal capability is reduced to zero.

Example: Setting UA = 0 after three minutes in the jacketed-CSTR case study simulates a complete cooling-system failure.

Zero-Emission Objective: An operational or strategic objective aimed at eliminating or substantially reducing greenhouse-gas and pollutant emissions through efficiency, electrification, renewable energy, process modification, hydrogen, and carbon capture.

Concluding Perspective

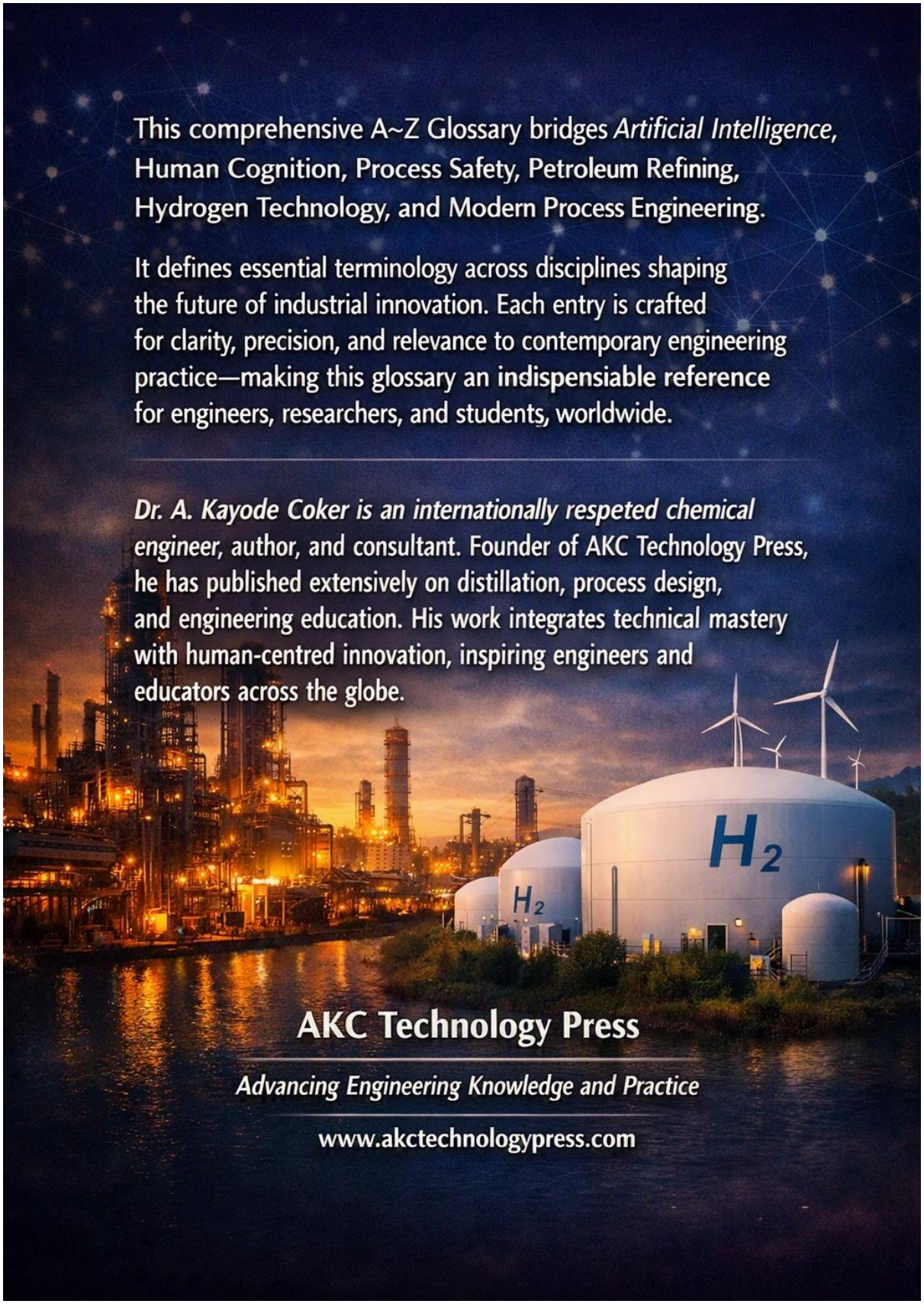
The terminology in this glossary demonstrates that modern chemical and process engineering increasingly combines several interconnected areas:

- Human intelligence and cognitive functions
- First-principles engineering knowledge
- Artificial intelligence and machine learning
- Process simulation and digital twins
- Process safety and functional safety
- Petroleum refining and crude-oil characterization
- Hydrogen manufacture and purification
- Greenhouse-gas management and CCUS
- Human-centered professional skills

AI provides computational speed, pattern recognition, prediction, data processing, and optimization. Process simulation and first-principles models provide physical and engineering foundations. Digital platforms connect plant data, models, and operational systems.

Human engineers remain responsible for engineering judgment, ethical reasoning, creativity, communication, leadership, contextual understanding, professional responsibility, and accountability.

Engineering excellence therefore depends on the effective integration of **Human Intelligence, Artificial Intelligence, Engineering Fundamentals, Process Safety, Digital Technology, and Human-Centered Skills**.


This comprehensive A~Z Glossary bridges *Artificial Intelligence*, Human Cognition, Process Safety, Petroleum Refining, Hydrogen Technology, and Modern Process Engineering.
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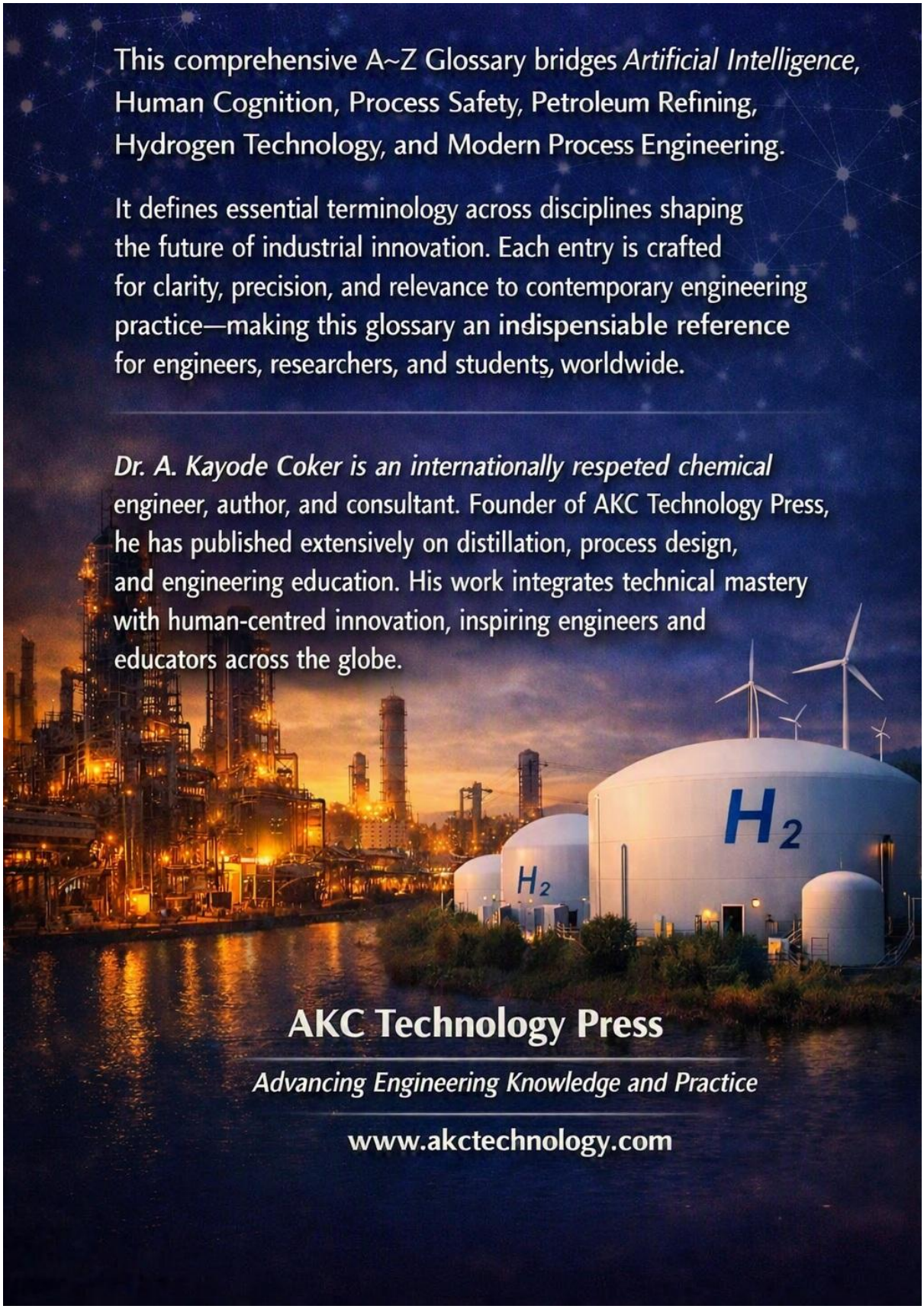
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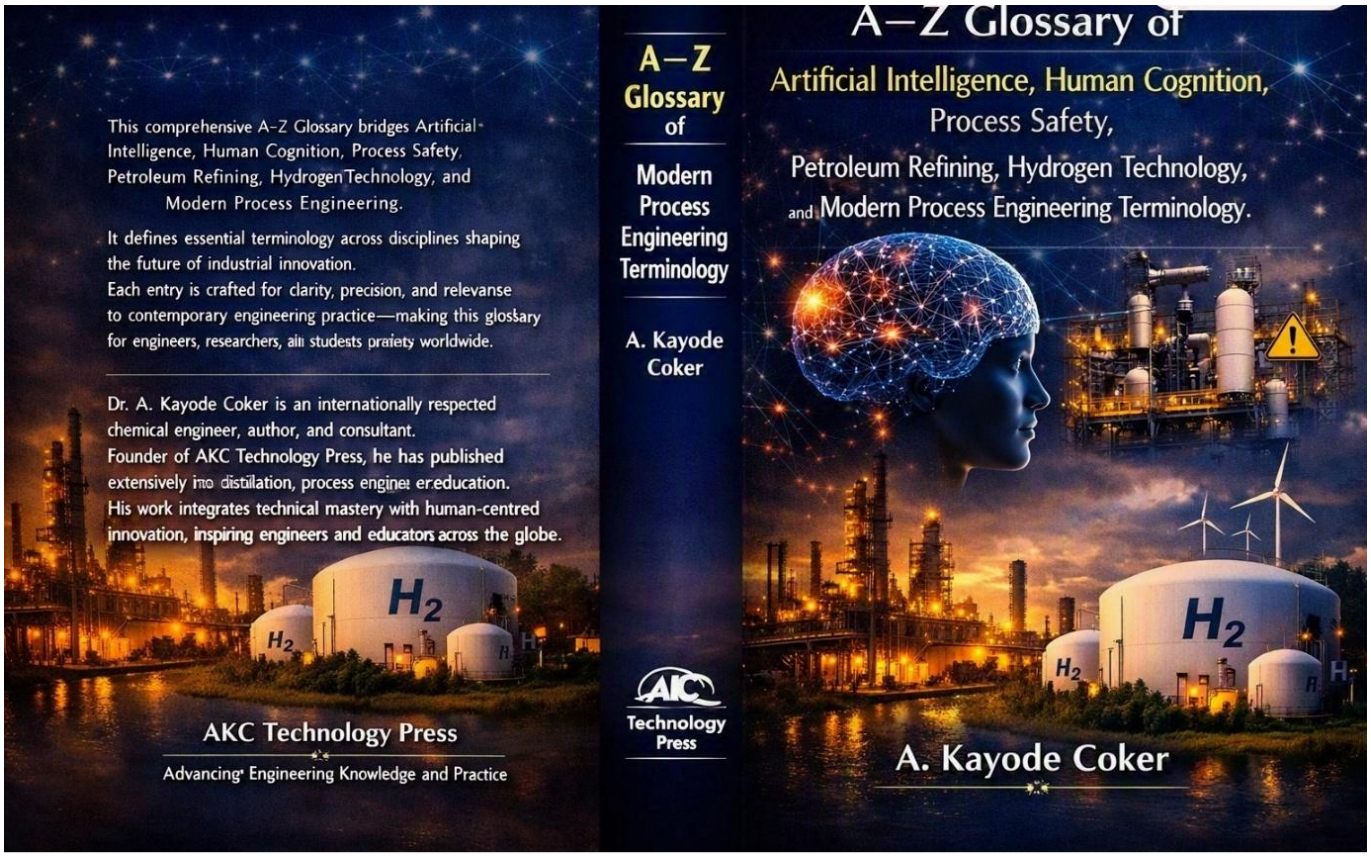
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Note: These downloadable Python scripts are intended for educational use; users are accountable for their implementation.

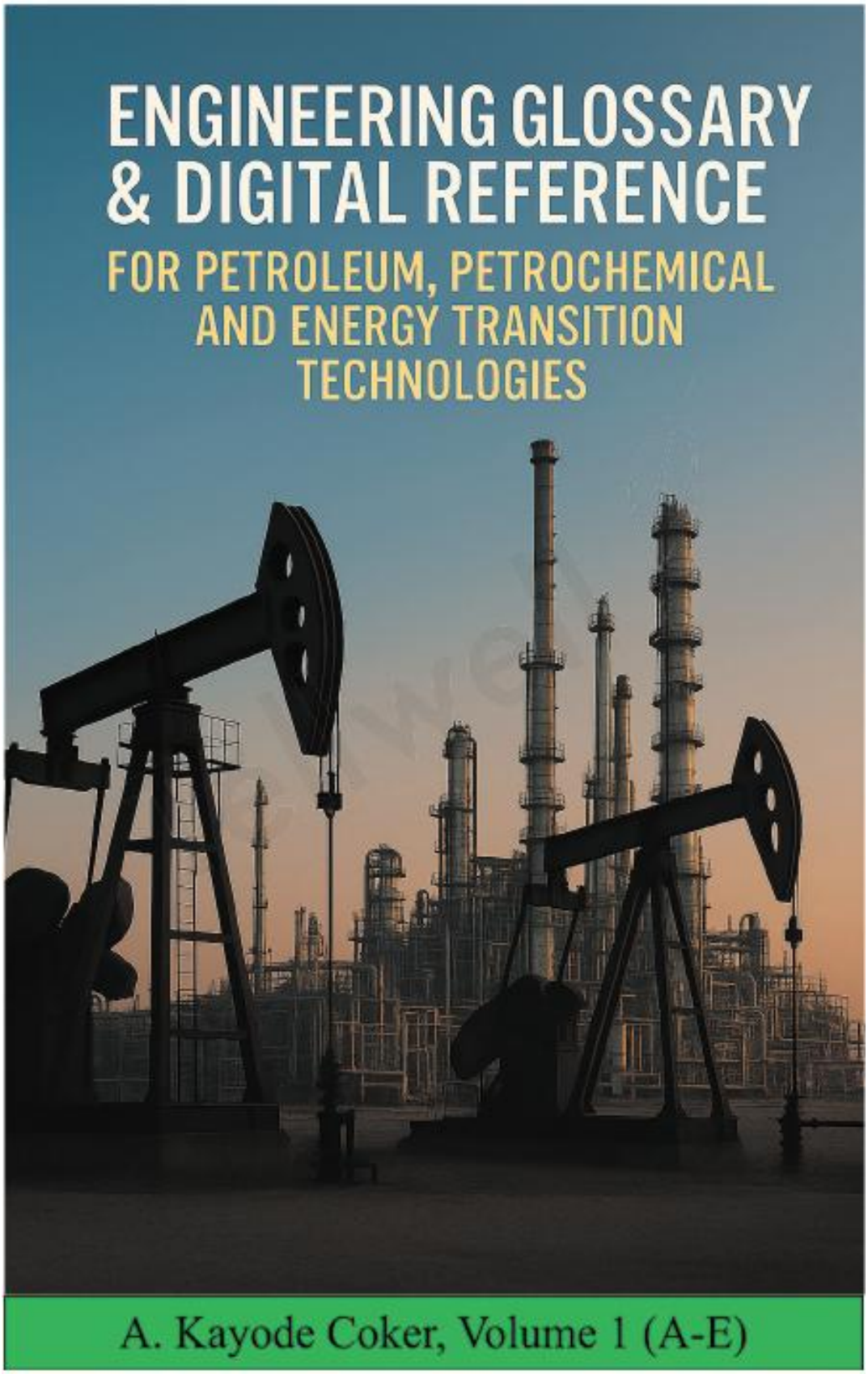
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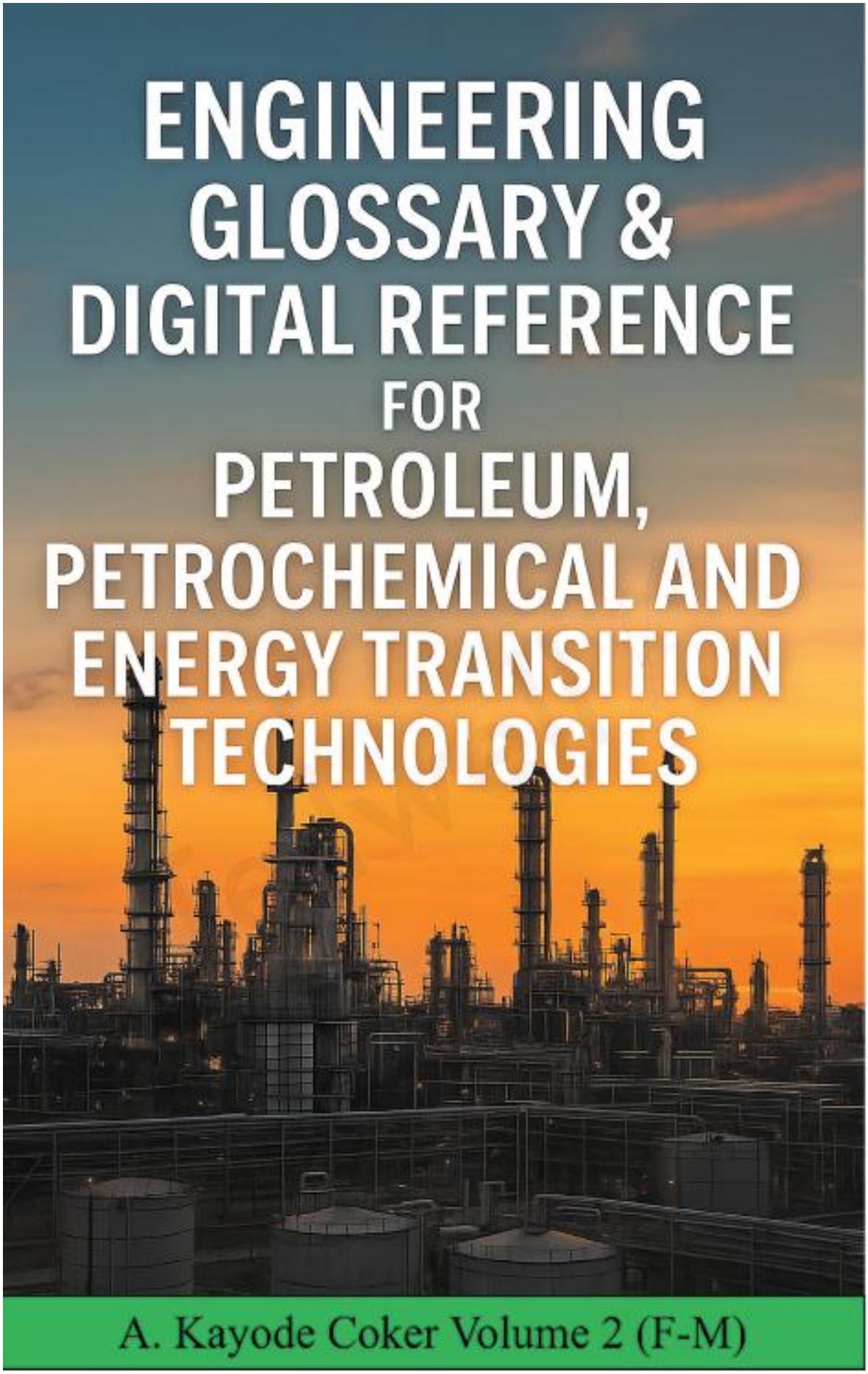
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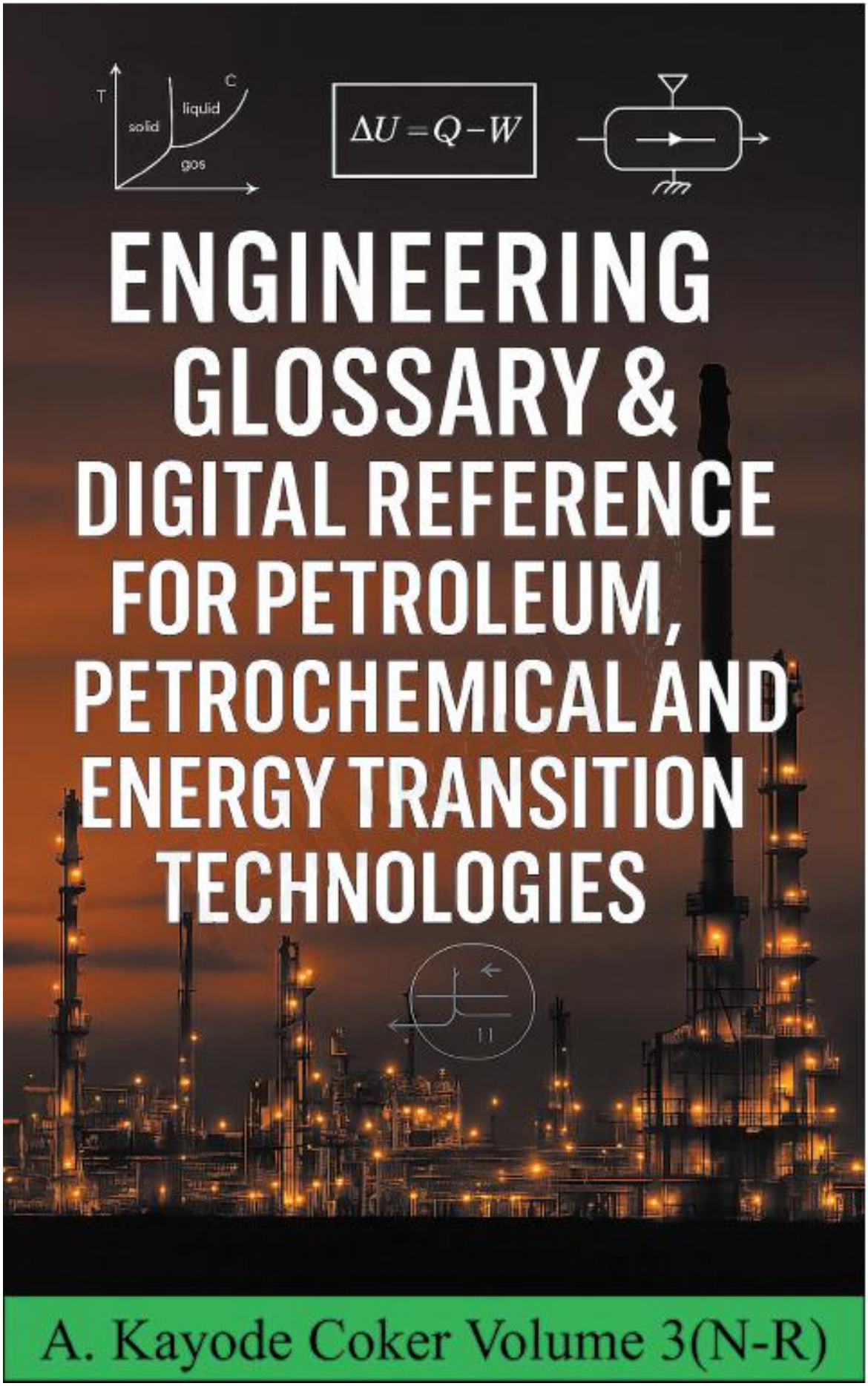

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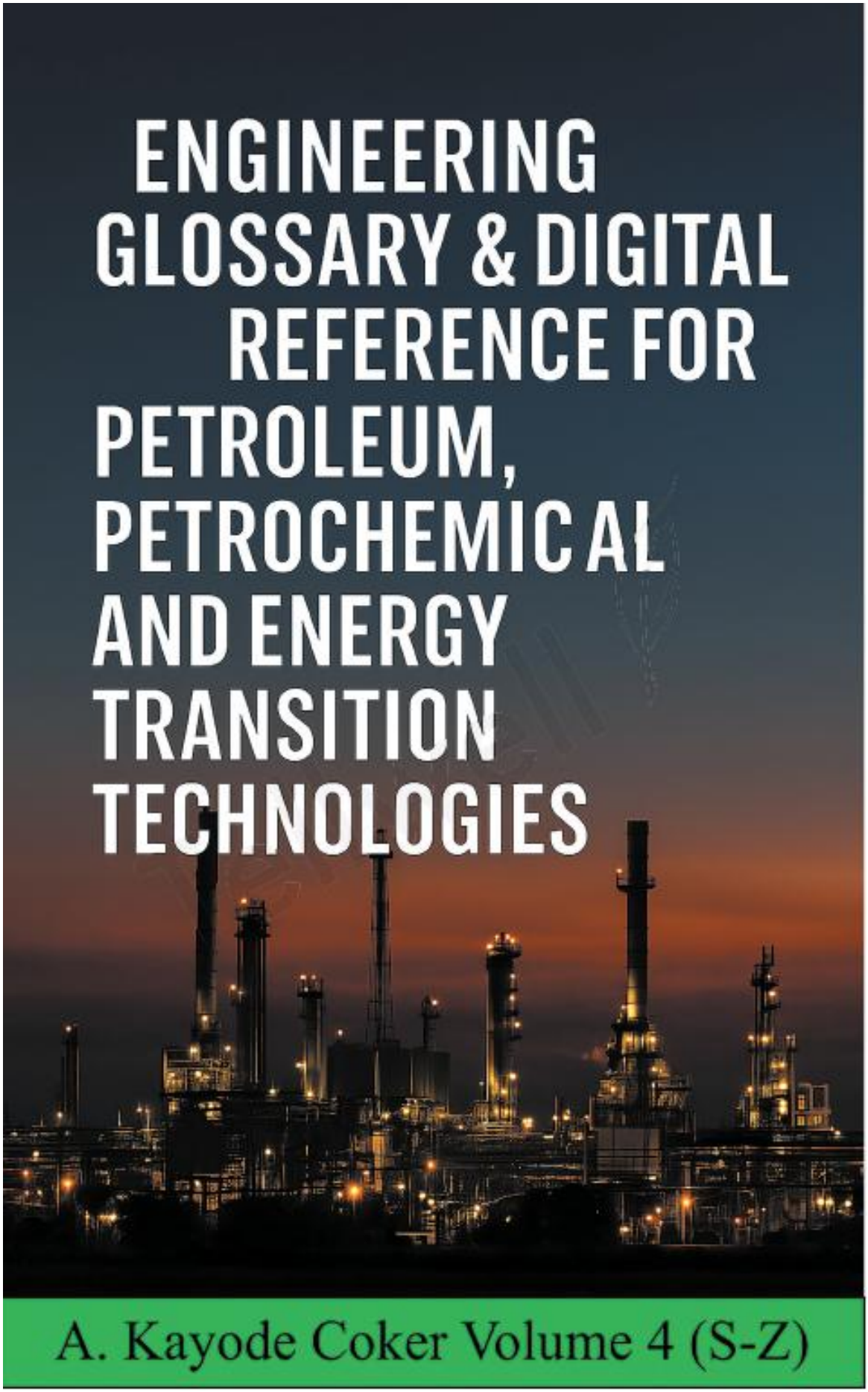

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