

UNIT 2

Fuel for Fuel Cells

- Fuel cells are devices that convert chemical energy into electrical energy through an electrochemical process. They are often considered a cleaner and more efficient alternative to traditional combustion-based power generation methods. The type of fuel used in a fuel cell depends on the specific design and intended application of the fuel cell system. Here are some common types of fuels used in fuel cells:
 1. Hydrogen (H_2): Hydrogen is the most common fuel for fuel cells, and it is often referred to as the "ideal" fuel for fuel cells because it produces electricity and water as the only byproducts when combined with oxygen. Hydrogen fuel cells are used in various applications, including transportation (hydrogen fuel cell vehicles), stationary power generation, and portable electronic devices.
 2. Methanol (CH_3OH): Methanol fuel cells, specifically direct methanol fuel cells (DMFCs), use methanol as a liquid fuel. They are commonly used in portable applications, such as laptop chargers and backup power supplies, due to the ease of handling and refueling with liquid methanol.
 3. Natural Gas: Some fuel cells can use natural gas as a fuel source. These are known as natural gas fuel cells or solid oxide fuel cells (SOFCs). They are often used for combined heat and power (CHP) applications, where both electricity and heat are generated simultaneously, making them suitable for residential and commercial buildings.

4. Propane (LPG): Propane fuel cells are similar to natural gas fuel cells but use propane as the fuel source. They can also be used for CHP (combined heat and power) applications and are often employed in off-grid or remote power generation.
 5. Ammonia (NH₃): Ammonia is another potential fuel for fuel cells, particularly in high-temperature solid oxide fuel cells. It is considered a promising option for clean energy production because it does not produce carbon dioxide (CO₂) when used as a fuel.
 6. Biomass-derived fuels: Some fuel cells can operate on biofuels produced from renewable sources, such as ethanol or biogas. These types of fuel cells are under development and hold promise for sustainable energy production.
 7. Synthetic Fuels: Researchers are exploring the use of synthetic fuels, such as synthetic hydrogen and hydrocarbons, as potential fuel sources for fuel cells. These synthetic fuels can be produced using renewable energy sources and carbon capture technology, reducing their environmental impact.
- The choice of fuel for a fuel cell system depends on factors such as the desired application, efficiency requirements, fuel availability and environmental considerations. Each type of fuel cell has its advantages and limitations, and ongoing research aims to improve fuel cell technology and explore new fuel options to advance clean and efficient energy generation

Hydrogen

- Hydrogen is a versatile and clean fuel source commonly used in fuel cells. Here are the details of hydrogen as a fuel for fuel cells:
- **1. Hydrogen Properties:**
- Hydrogen (H₂) is the lightest and most abundant element in the universe.
- It is odorless, colorless, and tasteless.
- Hydrogen has a high energy-to-weight ratio, making it an excellent fuel for various applications.
- **2. Hydrogen Production:**
- Hydrogen can be produced from various sources, including natural gas, water, biomass, and electrolysis.
- Steam Methane Reforming (SMR) is a common method to extract hydrogen from natural gas.
- Electrolysis splits water molecules into hydrogen and oxygen using electricity, often from renewable sources

- **3. Clean Energy:**

- Hydrogen fuel cells are considered clean energy technology because they produce electricity through an electrochemical reaction without combustion.
- The only byproduct of hydrogen fuel cell operation is water vapor (H₂O), making it environmentally friendly and reducing greenhouse gas emissions.

- **4. Efficiency:**

- Hydrogen fuel cells are highly efficient, with conversion efficiencies of 40% to 60% or even higher.
- They are more energy-efficient than internal combustion engines.

- **5. Applications:**

- **Transportation:** Hydrogen fuel cells are used in various vehicles, including cars (hydrogen fuel cell vehicles or FCVs), buses, trucks, and trains.
- **Stationary Power:** Hydrogen fuel cells can provide clean electricity and heat for residential, commercial, and industrial applications.
- **Portable and Backup Power:** Fuel cells are used in portable devices like laptops and as backup generators for critical infrastructure.

- **6. Challenges:**

- **Hydrogen Storage:** Storing hydrogen can be challenging due to its low density. Compressed gas, liquefaction, and solid-state storage methods are under development.
- **Infrastructure:** The development of a hydrogen infrastructure, including production, distribution, and refueling stations, is a significant challenge.
- **Cost:** Hydrogen fuel cells can be expensive to manufacture and deploy, although costs are decreasing with advancements in technology and scale.

- **7. Safety:**

- Hydrogen is flammable and has certain safety concerns, but modern hydrogen fuel systems are designed with safety in mind.
- Hydrogen is lighter than air and disperses quickly, reducing the risk of explosions.

- **8. Research and Advancements:**

- Ongoing research focuses on improving the efficiency and durability of hydrogen fuel cells.
- Advances in catalysts, membrane materials, and system design are continuously enhancing the technology.

- **9. Government Support:**

- Many governments around the world support hydrogen fuel cell technology through research funding, incentives, and policy initiatives to promote its adoption.
- Hydrogen as a fuel for fuel cells offers a promising pathway to a cleaner and more sustainable energy future, particularly when produced from renewable sources.

Hydrocarbon fuels

- Hydrocarbon fuels can be used in fuel cells, specifically in a type of fuel cell known as a "hydrocarbon fuel cell" or "hydrocarbon-fed fuel cell." These fuel cells enable the direct electrochemical conversion of hydrocarbon fuels into electricity.

1. Types of Hydrocarbon-Fed Fuel Cells:

- **Direct Methanol Fuel Cells (DMFCs):** DMFCs use methanol, a liquid hydrocarbon, as their primary fuel. They are commonly used in portable electronic devices, such as laptops and smartphones, due to the ease of handling and refueling with liquid methanol.
- **Solid Oxide Fuel Cells (SOFCs):** SOFCs can operate on various hydrocarbon fuels, including natural gas, propane, and methane. They are often used for stationary power generation and can reach high operating temperatures, making them versatile for different applications.
- **Molten Carbonate Fuel Cells (MCFCs):** MCFCs can use hydrocarbon fuels such as natural gas, methane, and even carbon dioxide. They are known for their high operating temperatures and are suitable for large-scale power generation.

- **2. Hydrocarbon Fuel Processing:**

- Hydrocarbon fuels must undergo a reforming or processing step to convert them into hydrogen-rich gas streams that can be used in the anode of fuel cells.
- Reforming methods include steam methane reforming (SMR) for natural gas and catalytic partial oxidation (CPOX) for liquid hydrocarbons like methanol.

- **3. Anode Reactions:**

- In hydrocarbon-fed fuel cells, the anode (negative electrode) is responsible for the oxidation of the hydrocarbon fuel.
- For example, in a DMFC, the anode reaction is:
- $\text{CH}_3\text{OH} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + 6\text{H}^+ + 6\text{e}^-$.

- **4. Advantages:**

- **Energy Density:** Hydrocarbon fuels have high energy densities, making them suitable for applications requiring long runtimes or high power output.
- **Storage and Transport:** Hydrocarbon fuels are relatively easy to store and transport compared to gaseous fuels like pure hydrogen.
- **Versatility:** Hydrocarbon-fed fuel cells can use existing hydrocarbon infrastructure and can be integrated into various energy systems.

- **5. Challenges:**

- **Carbon Formation:** The incomplete oxidation of hydrocarbons can lead to carbon deposition on the anode, which can reduce fuel cell performance.
- **Operating Temperature:** Some hydrocarbon-fed fuel cells, like SOFCs, operate at high temperatures, which can limit their suitability for certain applications.
- **Emissions:** The reforming process for hydrocarbon fuels can produce carbon dioxide (CO₂) emissions, although this can be mitigated through carbon capture technologies.

- **6. Applications:**

- Portable Devices: DMFCs are used in portable electronic devices, offering extended runtimes compared to traditional batteries.
- Stationary Power Generation: SOFCs and MCFCs can provide clean and efficient electricity for residential, commercial, and industrial applications.
- Combined Heat and Power (CHP): Some hydrocarbon-fed fuel cells are used for CHP systems, simultaneously producing electricity and heat for buildings.

- **7. Research and Development:**

- Ongoing research focuses on improving the efficiency, durability, and reliability of hydrocarbon-fed fuel cells.
- Efforts are also directed toward developing cleaner and more efficient hydrocarbon fuel processing technologies.
- Hydrocarbon-fed fuel cells provide an alternative to pure hydrogen fuel cells, allowing for the utilization of existing hydrocarbon infrastructure while offering cleaner and more efficient energy generation compared to traditional combustion-based systems. Continued advancements in fuel cell technology and hydrocarbon fuel processing are key to enhancing their performance and reducing their environmental impact.

Effect of impurities such as CO, S and others in fuel cells

- Impurities in fuel cells, such as carbon monoxide (CO), sulfur (S), and other contaminants, can have detrimental effects on fuel cell performance and durability. The impact of these impurities varies depending on the type of fuel cell and the specific impurity in question. Here's a breakdown of their effects:
- **1. Carbon Monoxide (CO):**
- **Effect:** CO is a common impurity in hydrogen-based fuel cells, particularly in reformed hydrogen obtained from hydrocarbon fuels. CO is known to poison catalysts and interfere with the electrochemical reactions occurring within the fuel cell.
- **Impact:** CO can reduce the overall efficiency of the fuel cell by blocking active sites on the catalyst, inhibiting the electrochemical oxidation of hydrogen, and decreasing power output.
- **Mitigation:** CO mitigation strategies include the use of CO-tolerant catalysts, improved fuel processing techniques to reduce CO levels, and the addition of CO oxidation catalysts in the anode compartment.

- **2. Sulfur (S) Compounds:**

- **Effect:** Sulfur impurities, such as hydrogen sulfide (H_2S) and sulfur dioxide (SO_2), can poison fuel cell components, particularly the catalysts and proton exchange membrane (PEM).
- **Impact:** Sulfur poisoning can lead to a significant reduction in fuel cell performance, decreased durability, and increased degradation rates. Sulfur compounds can chemically react with catalysts, leading to irreversible damage.
- **Mitigation:** Sulfur removal processes, such as desulfurization of fuel sources or the use of sulfur-tolerant catalysts, are employed to mitigate the impact of sulfur impurities. Hydrogen purification methods, like sulfur scrubbers, can be used to remove sulfur before it reaches the fuel cell.

- **3. Other Impurities:**

- **Water and CO₂:** Excessive moisture and carbon dioxide in the fuel stream can affect the performance of PEM fuel cells by interfering with the hydration of the membrane and affecting proton conductivity. Proper humidification and purification of the fuel stream are essential to maintain optimal conditions.
- **Particulate Matter:** Solid particulates or contaminants in the fuel can clog the flow channels and reduce the effectiveness of fuel cell components. Filtration and purification techniques are used to remove such impurities.
- **Heavy Metals:** Some impurities, such as heavy metals like lead and mercury, can poison catalysts and negatively impact fuel cell performance. Stringent quality control measures are necessary to ensure the purity of the fuel source.

- **4. Material and System Degradation:**

- Impurities can accelerate the degradation of materials within the fuel cell stack, leading to reduced lifespan and increased maintenance requirements.
- Degradation of fuel cell components can result from chemical reactions, physical interactions, and changes in material properties caused by impurities.
- Efforts to address the impact of impurities in fuel cells include the development of advanced materials, purification technologies, and control systems. Proper fuel processing, purification, and monitoring are crucial to maintaining fuel cell efficiency and longevity, especially when using hydrogen or reformat hydrogen as fuel sources. Researchers and engineers continue to work on improving fuel cell robustness and tolerance to impurities to make them more reliable in various applications.

- Fuel cell electrochemistry involves complex reactions occurring at the electrodes, which are critical for the generation of electricity in fuel cells. Electrode kinetics refers to the study of these electrode reactions, including the rates at which they occur and the factors influencing their kinetics. There are two primary reactions at the electrodes of fuel cells: the anode and the cathode.
- **1. Anode Electrode Kinetics:**
- At the anode, typically in hydrogen fuel cells, the primary reaction is the electrochemical oxidation of hydrogen:
 - Anode Reaction: $\text{H}_2 \rightarrow 2\text{H}^+ + 2\text{e}^-$
- This reaction involves the splitting of hydrogen molecules into protons (H^+) and electrons (e^-) on the anode catalyst surface.
- The kinetics of the anode reaction are influenced by several factors:
 - Catalyst Activity: The efficiency of the anode catalyst in promoting the hydrogen oxidation reaction.
 - Temperature: Higher temperatures generally lead to faster kinetics.
 - Hydrogen Concentration: A higher concentration of hydrogen at the anode increases reaction rates.
 - Catalyst Poisoning: Impurities or contaminants, such as carbon monoxide (CO), can inhibit the anode reaction.
 - Anode Surface Area: Larger surface areas provide more active sites for the reaction.

- **2. Cathode Electrode Kinetics:**

- At the cathode, the primary reaction in many fuel cells, including hydrogen fuel cells and direct methanol fuel cells, is the electrochemical reduction of oxygen:
 - Cathode Reaction: $\text{O}_2 + 4\text{H}^+ + 4\text{e}^- \rightarrow 2\text{H}_2\text{O}$
- This reaction involves the combination of oxygen molecules with protons and electrons to produce water.
- The kinetics of the cathode reaction are also influenced by various factors:
 - Catalyst Activity: The efficiency of the cathode catalyst in promoting the oxygen reduction reaction.
 - Temperature: Higher temperatures generally lead to faster kinetics.
 - Oxygen Concentration: A higher concentration of oxygen at the cathode increases reaction rates.
 - Catalyst Poisoning: Contaminants like carbon monoxide (CO) can inhibit the cathode reaction.
 - Cathode Surface Area: Larger surface areas provide more active sites for the reaction.

3. Rate-Determining Step:

- In many cases, the slowest step in the overall electrode reaction determines the overall rate of the fuel cell's electricity generation.
- The rate-determining step can vary depending on the specific fuel cell design, operating conditions, and catalyst materials.

4. Overpotential:

- Overpotential refers to the extra voltage or potential required to drive the electrode reaction faster than its thermodynamically preferred rate.
- Fuel cells typically operate with an applied voltage to overcome overpotential and ensure the desired reaction rates.
- Understanding and optimizing electrode kinetics are essential for improving the efficiency, performance, and durability of fuel cells. Researchers and engineers work **to develop catalyst materials and electrode designs** that minimize overpotential, enhance reaction rates, and reduce the impact of contaminants, ultimately leading to more efficient and practical fuel cell systems for various applications, including transportation, stationary power generation, and portable electronics.

- Electrode kinetics is a branch of electrochemistry that focuses on the study of the rates of electrochemical reactions occurring at electrode surfaces. These reactions are fundamental to a wide range of electrochemical devices, including batteries, fuel cells, electrochemical sensors, and electrolysis cells. Electrode kinetics involves understanding the mechanisms, kinetics, and factors that influence these reactions. Here are some key aspects of electrode kinetics:
- **1. Electrode Reactions:**
- Electrode kinetics primarily deals with two types of electrode reactions:
 - **Oxidation Reaction (Anodic Reaction):** This is the reaction that occurs at the anode (positive electrode), where electrons are released, and ions are oxidized.
 - **Reduction Reaction (Cathodic Reaction):** This is the reaction that occurs at the cathode (negative electrode), where electrons are consumed, and ions are reduced.
- **2. Reaction Mechanisms:**
- Understanding the detailed mechanisms of electrode reactions is essential for predicting and controlling their rates.
- Reaction mechanisms involve understanding the sequence of intermediate steps that occur during the overall electrode reaction.
- **3. Rate Equations:**
- Electrode kinetics aims to establish mathematical expressions (rate equations) that describe the relationship between the rate of the electrochemical reaction and factors such as electrode potential, concentration of reactants, temperature, and surface area.

- The Butler-Volmer equation is a fundamental relationship in electrochemistry that describes how the electrical current density (J) of a simple redox reaction at an electrode depends on the potential difference (overpotential, η) between the electrode and the electrolyte,

- **$J = J_0 [\exp(\alpha_a n F \eta / RT) - \exp(-\alpha_c n F \eta / RT)]$.**

It relates the anodic (oxidation) and cathodic (reduction) current densities to the potential, showing that the total current is the difference between the two. The equation is applicable to a wide range of potentials and can be used to extract exchange current density (J_0) and other kinetic parameters from polarization curves, though it has limitations when mass transport is significant.

J: Total current density **J_0 :** Exchange current density, representing the forward and reverse current at equilibrium

- **α_a, α_c :** Anodic and cathodic transfer coefficients, which are symmetry factors related to the activation energy for the respective reactions
- **n :** Number of electrons involved in the electron transfer step of the reaction
- **F :** Faraday's constant
- **R :** The universal gas constant
- **T :** The operating temperature
- **η (eta):** The overpotential, which is the difference between the applied voltage (V) and the equilibrium potential

The Butler-Volmer equation has a wide range of applications in various industries, including the modeling of batteries, the study of corrosion processes, and the optimization of industrial electrochemical processes.

The Tafel equation relates the overpotential of an electrode to the current density of an electrochemical reaction and is expressed as

$$\eta = a + b \log(i),$$

where η is the overpotential, i is the current density, and a and b are constants representing the Tafel intercept and Tafel slope.

It is a simplified version of the Butler – Volmer equation for conditions of high overpotential and is used to study electrode kinetics, determine corrosion rates and optimize processes like electroplating.

- **6. Factors Influencing Electrode Kinetics:**

- Several factors influence the rate of electrode reactions, including temperature, concentration of reactants, electrode material, surface area, and the presence of catalysts.

- **7. Application Areas:**

- Electrode kinetics is essential in the design and optimization of electrochemical devices, such as batteries, fuel cells, corrosion protection systems, and sensors.
- Understanding electrode kinetics is crucial for improving the efficiency, performance, and lifespan of electrochemical systems, as it allows researchers and engineers to design electrodes and operating conditions that maximize reaction rates while minimizing energy losses and unwanted side reactions.

Types of Voltage Losses

- In electrochemical systems like batteries, fuel cells, and electrochemical sensors, various types of voltage losses can occur, affecting the overall performance of the system. These voltage losses are often referred to as "voltage losses" or "voltage drops." Here are some common types of voltage losses in electrochemical systems:

1. Ohmic Losses (IR Losses):

1. Ohmic losses occur due to the resistance (R) of the electrolyte and the internal resistance of the cell components (e.g., electrodes, conductive materials).
2. These losses are described by Ohm's law: $V = IR$, where V is the voltage drop, I is the current, and R is the resistance.
3. Ohmic losses can reduce the efficiency of the system and result in heating of the components.

2. Activation Overpotential ($\eta_{\text{activation}}$):

1. Activation overpotential is the energy barrier that must be overcome for an electrochemical reaction to occur at the electrode-electrolyte interface.
2. It is influenced by the kinetics of the electrode reactions and can be described by the Butler-Volmer equation or Tafel equation.
3. Activation overpotential increases with higher reaction rates or when the electrode surface is less catalytic.

- **Concentration Overpotential ($\eta_{\text{concentration}}$):**

- Concentration overpotential arises from the variation in reactant concentrations near the electrode surface.
- It can occur when the rate of mass transport of reactants to the electrode surface is slower than the rate of electrochemical reactions.
- Concentration overpotential can be reduced by improving mass transport through methods such as better electrolyte flow or electrode design.

- **Ohmic Drop in Electrolyte (IR Loss in Electrolyte):**

- In addition to the internal resistance of cell components, there can be resistance within the bulk of the electrolyte.
- This type of resistance can lead to voltage losses in the electrolyte and reduce the overall cell performance.

- **Charge Transfer Resistance (R_{ct}):**

- Charge transfer resistance represents the resistance to the flow of charge at the electrode-electrolyte interface.

- It is related to the activation overpotential and can be affected by factors such as electrode materials and the presence of catalysts.

- Reducing charge transfer resistance is critical for improving the kinetics of electrode reactions.

- **Mass Transport Limitations:**

- Mass transport limitations occur when the rate at which reactants are transported to or from the electrode surface is slower than the rate of the electrochemical reaction.

- This limitation can result in concentration overpotential and reduced cell performance.

Electrode Geometry and Configuration Losses:

The geometric design and configuration of the electrodes can also contribute to voltage losses. For example, poorly designed electrode structures can lead to non-uniform current distribution and increased resistive losses.

- Understanding and minimizing these voltage losses is crucial for optimizing the efficiency and performance of electrochemical systems. Researchers and engineers often work to mitigate these losses through improved materials, electrode designs, and operating conditions.

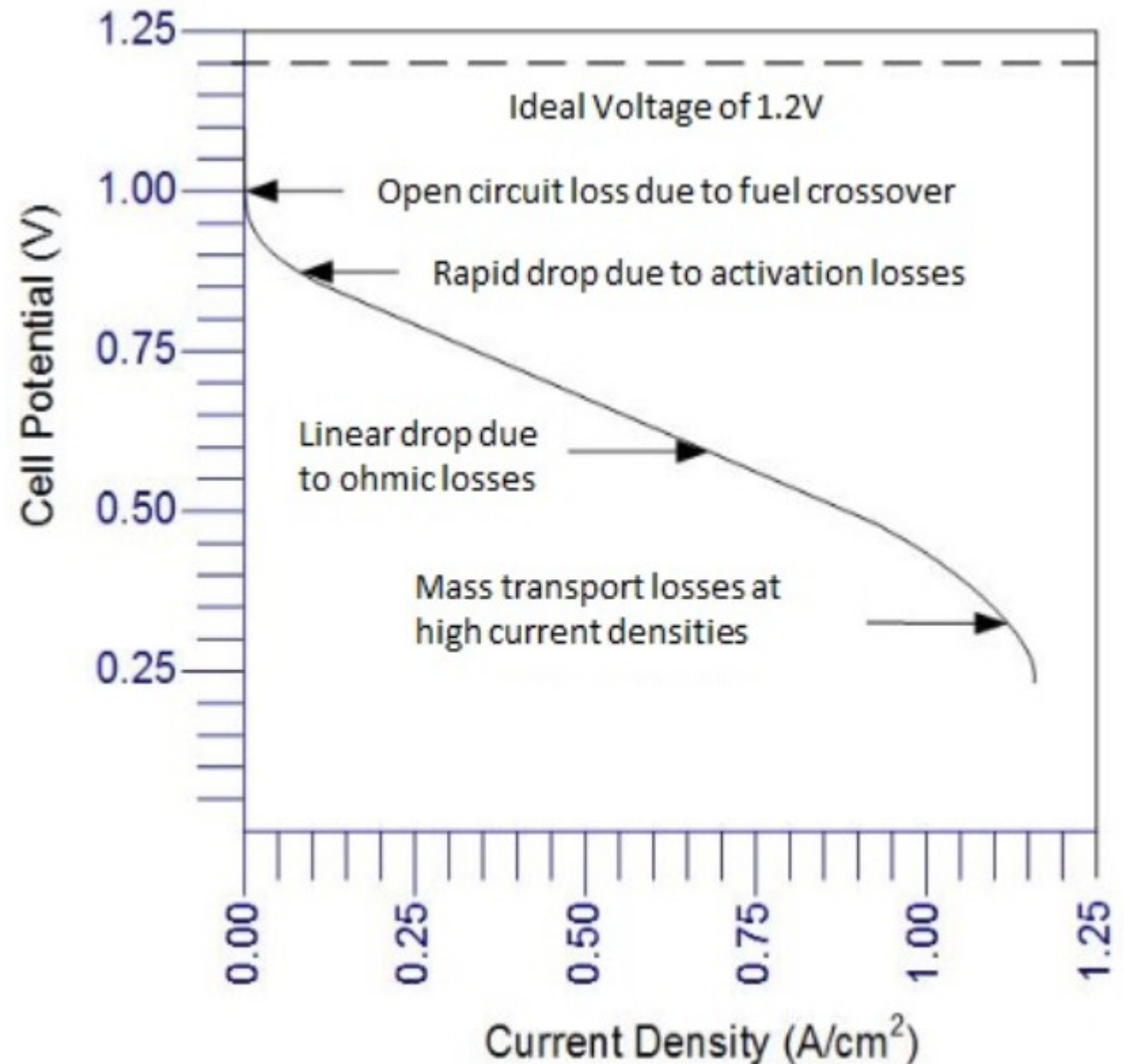
Polarization

The chemical action that occurs in the cell while the current is flowing causes hydrogen bubbles to form on the surface of the anode. This action is called polarization. Some hydrogen bubbles rise to the surface of the electrolyte and escape into the air, some remain on the surface of the anode.

Polarization Losses:

Polarization losses refer to the overall reduction in voltage or potential difference between the electrodes and are often due to a combination of activation overpotential, concentration overpotential, and ohmic losses.

These losses are typically measured as a difference between the open-circuit voltage (OCV) and the actual cell voltage under load.



efficiency is simply the practical cell-output voltage divided by the thermodynamically reversible voltage at the stated temperature and pressure of operation. This indicates how much free energy is lost by inefficiencies in operating the fuel cell stack, without regard to how much of the enthalpy of the reaction is liberated as heat (the $T\Delta S$ term).

Fuel cell efficiency directly impacts the operating cost as well as fuel storage requirements. In mobile applications, the efficiency becomes even more important because the fuel must be moved with the cell. A less efficient fuel cell must move fuel to travel the same distance, thus wastes some of the generated energy moving the additional fuel. One major advantage of fuel cells becomes apparent when we compare their efficiencies to the efficiency of the internal combustion engine. The typical efficiency of an internal combustion engine is on the order of 20%. Thus, to power a vehicle with the same performance and range, we only need to carry half as much fuel, assuming a 40% efficient [PEM](#) cell stack.

Fuel Cell Type	Efficiency
Alkaline	70%
Molten carbonate	60–80% with cogeneration
Phosphoric acid	40–80% with cogeneration
Solid oxide	60%
Proton exchange membrane	40–50%

- **Hydrogen Tank (H₂ Tank)**
 - Stores compressed hydrogen gas onboard the vehicle.
 - Hydrogen is supplied from external renewable sources (like wind-powered hydrogen production shown here).
- **Fuel Cell**
 - Core unit that converts chemical energy into electricity.
 - Inside the fuel cell:
 - Hydrogen (H₂) enters the anode.
 - Oxygen (O₂) from air enters the cathode.
 - Through an electrochemical reaction (not combustion), H₂ is split into protons (H⁺) and electrons (e⁻).
 - Protons pass through a membrane; electrons flow through an external circuit, producing **electricity**.
 - At the cathode, protons, electrons, and oxygen combine to form **water (H₂O)** as the only byproduct.
- **Battery**
 - Stores excess electricity generated by the fuel cell.
 - Provides extra power during acceleration and stores regenerative braking energy.
- **Controller**
 - Manages the power flow between the fuel cell, battery, and motor to ensure efficient operation.
- **Electric Motor**
 - Uses electricity to drive the vehicle's wheels.
 - Provides smooth, quiet, and zero-emission propulsion.
- **Inputs and Outputs:**
 - **Inputs:** Hydrogen (H₂) from the onboard tank and Oxygen (O₂) from the air.
 - **Outputs:** **Electricity** (to power the motor). **Water (H₂O vapor)** as the only emission.

Hydrogen fuel cell electric vehicle (FCEV)

