

Material Properties of Copper Oxychloride and Their Importance in the Thermolysis Step of the Cu–Cl Hydrogen Production Cycle

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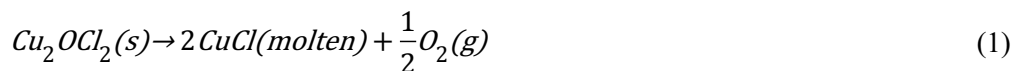
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Abstract - The Copper–Chlorine (Cu–Cl) thermochemical cycle is a leading candidate for large-scale, clean hydrogen production, offering the advantage of relatively low operating temperatures compared to other cycles. Within this process, the thermolysis step—where copper oxychloride (Cu_2OCl_2) decomposes into copper(I) chloride (CuCl) and oxygen gas—is both thermodynamically critical and operationally demanding. Despite its importance, there is limited consolidated data on the material behavior of Cu_2OCl_2 under high-temperature conditions. This paper presents a comprehensive study of the chemical, physical, thermal, mechanical, thermodynamic, and kinetic properties of Cu_2OCl_2 and their relevance to the thermolysis step. Key properties such as thermal decomposition range (500–530 °C), specific heat capacity (~0.45 J/g·K), thermal conductivity (~0.48 W/m·K), bulk density (~2.1 g/cm³), and activation energy (~100–120 kJ/mol) are examined. The paper also addresses phase stability, material reactivity with common reactor linings, particle size distribution, and handling considerations including toxicity and attrition. Each property is evaluated in terms of its impact on reactor design, energy integration, process reliability, and safety. By focusing on the material characteristics of Cu_2OCl_2 , this study fills a critical knowledge gap in the Cu–Cl cycle literature. It provides engineers and researchers with the data needed to improve thermolysis reactor performance and develop scalable, energy-efficient systems for hydrogen production. The findings serve as a foundation for optimizing material selection, process conditions, and reactor configurations in future implementations of the Cu–Cl thermochemical cycle.

Keywords: Cu-Cl cycle; copper oxychloride; material properties; thermolysis reaction; hydrogen production.

1. Introduction

The thermolysis reaction in the Copper-Chlorine (Cu-Cl) cycle is a key step in a thermochemical process for sustainable hydrogen production, occurring at approximately 550°C. In this endothermic reaction, copper oxychloride (Cu_2OCl_2 , solid) decomposes into copper(I) chloride (CuCl , molten) and oxygen gas (O_2 , gas), as described by the equation [1], [2], [3], [4], [5], [6]:



The materials involved in this reaction are

- Reactant: Copper oxychloride (Cu_2OCl_2 , solid).
- Products: Copper(I) chloride (CuCl , molten), Oxygen (O_2 , gas).

With an enthalpy change of 120–150 kJ/mol, this reaction produces oxygen as a valuable byproduct while generating CuCl for the subsequent electrolysis step, closing the cycle [7], [8]. Reactor design must account for solid handling of Cu_2OCl_2 and CuCl , efficient heat transfers due to the high temperature, and safe venting of hot O_2 gas [6], [9], [10], [11]. Conducted in fluidized or packed-bed reactors, thermolysis requires precise temperature control and efficient material handling to optimize energy use and ensure high yields. Integrated with high-temperature heat sources like nuclear or solar thermal energy, this reaction is critical for scalable, efficient, and environmentally friendly hydrogen production [5], [9], [10], [12].

While numerous studies have explored the Cu–Cl thermochemical cycle from a process or systems perspective, there remains a critical gap in the literature regarding the material-specific evaluation of the thermolysis step—particularly concerning Copper Oxychloride (Cu_2OCl_2) and its behavior under high-temperature conditions. Most existing work focuses

on overall cycle efficiency, system integration with solar or nuclear heat sources, or kinetics of the complete cycle. However, the thermolysis step, which operates at the highest temperature in the cycle (~500–530 °C), involves unique materials and thermal conditions that pose challenges for Reactor design and heat transfer, material degradation and compatibility, and product separation and recovery. There is limited consolidated data on how the chemical, thermal, and mechanical properties of Cu_2OCl_2 , CuCl , and O_2 interact under these specific conditions.

This paper fills that gap by providing a comprehensive analysis of all properties of the materials involved in the thermolysis step of the Copper–Chlorine (Cu–Cl) thermochemical cycle for hydrogen production in addition to the importance of these properties in the Cu–Cl cycle. The paper specifically aims to examine chemical, physical, thermal, mechanical, thermodynamic and kinetic properties of the reactant and products materials of the thermolysis process. By offering a material-centric perspective on the thermolysis step, this paper provides targeted guidance for engineers, researchers, and system designers seeking to optimize Cu–Cl cycle performance at the material and reactor level.

2. Properties of the Copper Oxychloride (Cu_2OCl_2) - Solid Reactant

2.1. Chemical Properties

Copper oxychloride (Cu_2OCl_2) is the key solid reactant in the thermolysis step of the Cu–Cl cycle, where it decomposes thermally at high temperatures (~500–530 °C) to produce copper(I) chloride (CuCl) and oxygen gas (O_2). Its chemical behavior under these conditions determines the reaction's efficiency, selectivity, and operational stability. The main chemical properties of Cu_2OCl_2 relevant to this step include:

2.1.1. Thermal Decomposition Behavior:

Copper oxychloride (Cu_2OCl_2) undergoes a well-defined thermal decomposition in the temperature range of approximately 500–530 °C as shown in equation (1). This endothermic reaction is a core component of the Cu–Cl cycle's thermolysis step, responsible for generating oxygen gas and recyclable copper(I) chloride (CuCl), which feeds directly into the electrolysis stage.

Experimental studies have confirmed that Cu_2OCl_2 remains stable as a solid up to this decomposition temperature range, after which it decomposes predictably and completely under controlled conditions [8], [13], [14], [15]. The decomposition is accompanied by an enthalpy change in the range of 120–150 kJ/mol, requiring a significant but manageable thermal energy input, especially when integrated with high-temperature heat sources like nuclear or concentrated solar thermal energy [16], [17], [18], [19].

Importance in the Cu–Cl Cycle

Understanding and controlling the thermal decomposition behavior of Cu_2OCl_2 is essential for the efficiency, safety, and scalability of the Cu–Cl hydrogen production process:

1. **Temperature Sensitivity and Control:** Cu_2OCl_2 decomposes in a narrow range (~500–530 °C), allowing precise temperature control in the reactor. This helps ensure complete conversion without damaging the reactor or forming unwanted by-products [8], [20], [21].
2. **Reaction Predictability:** Its predictable solid-state decomposition supports stable kinetics and reliable system performance. This enables the design of reactors with accurate heating profiles, residence times, and safe venting systems [10], [22].
3. **Energy Planning and Integration:** The known enthalpy change (120–150 kJ/mol) makes it suitable for integration with solar or nuclear heat sources. This supports energy-efficient hydrogen production [8].
4. **Efficient Phase Separation:** The reaction yields molten CuCl and gaseous O_2 , facilitating easy separation and downstream handling without complex purification steps [10].
5. **Reactor Compatibility:** Since Cu_2OCl_2 does not melt or sublime, it remains suitable for use in fluidized or packed-bed reactors, preserving material structure and process integrity [14], [23].
6. **System Reliability and Safety:** Accurate thermal behavior data helps prevent under- or over-heating, which could lead to incomplete reactions, equipment damage, or safety hazards.

2.1.2. Phase and Purity:

Cu_2OCl_2 exists as a monoclinic crystalline solid under normal and elevated temperatures up to its decomposition point. This well-defined crystalline structure promotes consistent thermal behavior and ensures uniform heat absorption throughout the particle bed [24].

The purity of Cu_2OCl_2 used in the thermolysis step is typically greater than 98% [8]. High purity is critical because impurities such as unreacted CuCl_2 or CuO can catalyze side reactions, disrupt reaction kinetics, and generate unwanted by-products or residues. These effects can reduce the yield of CuCl and O_2 , necessitate frequent reactor maintenance, and decrease the overall process efficiency [25], [26], [27].

Additionally, impurities may affect the melting behavior or cause localized sintering, which can impact particle flow in fluidized beds and increase the risk of reactor fouling or clogging. Uniform phase and high purity are thus essential for reliable performance, reactor longevity, and predictable thermal decomposition.

Importance in the Cu-Cl Cycle

1. **High Yield Maintenance:** High purity minimizes side reactions, ensuring maximum production of CuCl and O_2 , which is essential for the cycle's efficiency and hydrogen output [8]. This directly impacts the overall productivity of the process.
2. **Reactor Longevity:** Reduced impurities prevent residue buildup, decreasing the frequency of reactor cleaning and extending equipment lifespan [25]. This reduces downtime and maintenance costs.
3. **Consistent Kinetics:** The monoclinic crystal structure ensures uniform decomposition behavior, supporting stable reaction kinetics and reliable process performance [24].
4. **Prevention of Fouling:** High purity avoids sintering or clogging in fluidized beds, maintaining smooth particle flow and operational continuity [28].
5. **Process Efficiency:** Consistent phase behavior minimizes energy losses from side reactions or incomplete decomposition, optimizing energy use in the cycle [10].
6. **Safety Enhancement:** Minimized impurities reduce the risk of unexpected reactions, enhancing worker safety and operational stability [29].

2.1.3. Chemical Stability:

Cu_2OCl_2 exhibits robust chemical stability as a solid up to its decomposition temperature of 500–530°C, showing no tendency to oxidize, hydrolyze, or degrade under inert or ambient atmospheric conditions [20]. This stability ensures that the material can be safely stored, preheated, and transferred without premature reactions or energy losses, which is critical for maintaining process efficiency. The lack of reactivity with surrounding gases or reactor materials minimizes the risk of contamination or side reactions, preserving the purity of the products (CuCl and O_2) and extending the operational life of reactor components. This property is particularly valuable in large-scale thermochemical operations, where unstable materials could lead to energy inefficiencies, unexpected maintenance, or safety hazards. The chemical stability of Cu_2OCl_2 supports predictable decomposition pathways, ensuring consistent reaction outcomes and facilitating integration with high-temperature heat sources [10]. By preventing unintended chemical interactions, this property enhances the reliability, safety, and scalability of the Cu-Cl cycle for industrial hydrogen production[15].

Importance in the Cu-Cl Cycle

1. **Safe Material Handling:** Chemical stability allows for safe storage and transfer of Cu_2OCl_2 , reducing the risk of premature reactions and ensuring worker safety during handling [20].
2. **Minimized Side Reactions:** Low reactivity with gases or reactor materials ensures a predictable decomposition pathway, maintaining product purity and process efficiency [10].
3. **Reactor Durability:** Stability prevents corrosion or material interactions, extending the operational life of reactor components and reducing maintenance costs [8].

4. **Energy Optimization:** By preventing energy losses from unintended reactions, chemical stability enhances the efficient use of thermal energy inputs, supporting sustainable operation [10].
5. **Process Reliability:** Consistent chemical behavior supports stable and predictable operation, critical for achieving reliable performance in industrial-scale hydrogen production [8].
6. **Safety Assurance:** Reduced risk of unexpected reactions enhances overall process safety, protecting both workers and equipment from hazardous conditions [29].

2.1.4. Reactivity with Other Materials:

Cu_2OCl_2 demonstrates low chemical reactivity with a wide range of materials commonly used in high-temperature reactor construction, such as quartz, alumina, zirconia, and ceramic linings, at 500–530°C [10]. This inert behavior is crucial for maintaining reactor integrity under the high-temperature conditions of the thermolysis step, where material interactions could lead to corrosion, fouling, or secondary reactions. The low reactivity ensures that Cu_2OCl_2 does not degrade reactor components or contaminate the reaction products, preserving the purity of CuCl and O_2 . This property simplifies reactor material selection, allowing the use of standard refractory materials without the need for specialized coatings or linings. By minimizing chemical interactions, Cu_2OCl_2 supports long-term operational stability, reduces maintenance requirements, and enhances the safety of the thermolysis process. This characteristic is particularly important for industrial-scale applications, where reactor durability and product quality are critical for economic viability and process reliability [8], [30].

Importance in the Cu-Cl Cycle

1. **Reactor Longevity:** Low reactivity prevents corrosion of reactor materials, significantly extending equipment lifespan and reducing replacement costs, which enhances economic viability [10].
2. **Process Purity:** Minimized interactions with reactor materials ensure high purity of CuCl and O_2 , critical for downstream processes and overall cycle efficiency [8].
3. **Operational Stability:** Reduced fouling or sticking maintains consistent reactor performance, minimizing disruptions and ensuring continuous operation [28].
4. **Cost Efficiency:** Decreased maintenance and material replacement needs lower operational costs, making the Cu-Cl cycle more economically feasible [10].
5. **Safety:** Preventing hazardous material interactions reduces risks of equipment failure or safety incidents, enhancing overall process safety [29].
6. **Simplified Reactor Design:** Inert behavior allows the use of standard refractory materials, simplifying reactor construction and reducing design costs for large-scale applications [10].

2.1.5. Formation and Decomposition Pathway

Cu_2OCl_2 is formed in earlier steps of the Cu-Cl cycle through reactions involving copper and chlorine compounds, typically in a controlled chemical environment, and decomposes predictably at 500–530°C into CuCl and O_2 without forming intermediate phases. This direct decomposition pathway is a key feature of the thermolysis step, ensuring a straightforward reaction that minimizes complexity in reactor design and operation. The absence of side reactions or byproducts simplifies product recovery, as the CuCl and gaseous O_2 can be easily separated without additional purification steps. The predictable formation and decomposition of Cu_2OCl_2 support consistent reaction kinetics, enabling precise control over the thermolysis process. This property is critical for maintaining high conversion efficiencies and integrating the process with high-temperature heat sources, such as nuclear or solar thermal energy, for sustainable hydrogen production. The straightforward pathway also enhances the scalability of the Cu-Cl cycle, as it reduces the risk of process disruptions and supports reliable operation in industrial settings [8], [31], [32], [33].

Importance in the Cu-Cl Cycle

1. **Simplified Process Design:** The direct decomposition pathway eliminates the need for additional separation or purification steps, streamlining the thermolysis process and reducing operational complexity [10].

2. High Efficiency: Predictable decomposition ensures maximum conversion to CuCl and O₂, optimizing hydrogen production efficiency and minimizing material waste [8].
3. Energy Savings: Avoiding side reactions or intermediate phases reduces energy losses, enhancing the overall energy efficiency of the thermolysis step [25].
4. Reactor Stability: Consistent decomposition supports stable reactor operation, minimizing fluctuations in performance and ensuring reliable product yields [28].
5. Scalability: The straightforward pathway facilitates scaling up the process for industrial applications, ensuring consistent performance in large-scale hydrogen production systems [8].
6. Safety: Reduced risk of unexpected reactions enhances operational safety, protecting workers and equipment from hazardous conditions [29].

2.1.6. Toxicity and Chemical Handling

Cu₂OCl₂ exhibits low toxicity, but careful handling is required to prevent dust inhalation, which can pose health risks to workers [29]. Proper containment systems, such as sealed transport mechanisms and adequate ventilation, are essential to ensure safe storage, transfer, and processing of the material. These measures protect personnel from potential respiratory hazards and prevent dust accumulation that could foul reactor components. The low toxicity of Cu₂OCl₂ makes it relatively safe for industrial use, provided that appropriate handling protocols are followed. This property simplifies the implementation of safety measures, reducing the need for extensive protective equipment while maintaining compliance with occupational health standards. Effective handling also preserves the material's integrity, ensuring consistent decomposition behavior and preventing contamination of the reaction products. This characteristic is crucial for maintaining operational continuity, protecting equipment, and supporting the scalability of the Cu-Cl cycle for large-scale hydrogen production [10], [34].

Importance in the Cu-Cl Cycle

1. Worker Safety: Low toxicity, combined with proper containment, minimizes health risks, ensuring a safe working environment for personnel handling Cu₂OCl₂ [29].
2. Equipment Protection: Dust control prevents fouling or clogging of reactor components, extending equipment lifespan and reducing maintenance requirements [10].
3. Regulatory Compliance: Adherence to safe handling protocols ensures compliance with occupational health and safety standards, avoiding legal or operational issues [29].
4. Operational Continuity: Effective handling minimizes downtime from health or equipment issues, maintaining consistent process performance and productivity [10].
5. Cost Efficiency: Reduced health risks and equipment maintenance needs lower liability and operational costs, improving the economic viability of the Cu-Cl cycle [29].
6. Process Reliability: Proper handling preserves material integrity, ensuring consistent decomposition behavior and reliable performance across the thermolysis step [8].

2.2 Physical Properties

Cu₂OCl₂ remains a solid with a density of ~4.3 g/cm³, particle size of 50–200 μm, and greenish-yellow color, facilitating compact reactor loading, efficient heat transfer, and easy identification [8], [24]. These properties ensure smooth handling in fluidized or packed-bed reactors, optimize reaction kinetics through increased surface area, and support quality control, enhancing operational efficiency and scalability.

2.2.1. Phase Stability:

Copper oxychloride (Cu₂OCl₂) maintains its solid phase up to its decomposition temperature range of 500–530°C, exhibiting no tendency to melt or sublime under the high-temperature conditions of the thermolysis step [24], [35], [36]. This phase stability is a fundamental property that ensures Cu₂OCl₂ remains structurally intact during handling, transport, and reaction, making it ideal for processing in fluidized or packed-bed reactors commonly used in the Cu-Cl cycle. By remaining solid, Cu₂OCl₂ avoids complications such as sticking, clogging, or material loss that could arise from molten or

gaseous phases, ensuring smooth material flow and consistent reaction conditions. This property simplifies reactor design by eliminating the need for specialized equipment to manage phase transitions, thereby reducing construction and operational costs. The solid-state stability also promotes uniform heat distribution across the reactor bed, which is critical for achieving predictable decomposition kinetics and high reaction yields. This characteristic is particularly advantageous for industrial-scale applications, as it supports the use of standard solid-handling systems and enhances process scalability, reliability, and efficiency [10]. Furthermore, the absence of phase changes reduces energy requirements, aligning with the cycle's goal of sustainable hydrogen production[13], [27].

Importance in the Cu-Cl Cycle

1. **Efficient Solid Handling:** The solid phase enables straightforward transport and processing in reactors, reducing operational complexity and ensuring smooth material flow, critical for continuous large-scale operations [10].
2. **Simplified Reactor Design:** Avoiding melting or sublimation makes Cu_2OCl_2 compatible with standard fluidized or packed-bed reactors, lowering design and construction costs and facilitating industrial implementation [28].
3. **Process Stability:** Maintaining a solid state ensures consistent reaction conditions, minimizing variations in kinetics and enhancing process reliability across multiple cycles [24].
4. **Energy Efficiency:** The absence of phase changes eliminates energy requirements for managing melting or vaporization, optimizing heat utilization and reducing the energy footprint of the thermolysis step [8].
5. **Safety Assurance:** Solid-state stability prevents issues like reactor fouling from molten material, reducing risks of equipment damage and enhancing operational safety for workers and systems [29].
6. **Scalability for Industrial Applications:** Handling Cu_2OCl_2 as a solid supports the design of large-scale reactors, ensuring consistent performance and facilitating industrial hydrogen production [10].

2.2.2. Density:

Cu_2OCl_2 possesses a density of approximately 4.3 g/cm^3 at 550°C , a critical property that influences reactor fill volume, material handling, and heat distribution within the solid bed during the thermolysis step [4], [7], [24], [37]. This high density allows for compact reactor loading, maximizing space utilization and enabling efficient processing of large quantities of material in a limited volume. In fluidized or packed-bed reactors, the density of Cu_2OCl_2 governs particle flow dynamics, ensuring stable fluidization and uniform heat transfer, which are essential for consistent decomposition. The high density also enhances heat retention within the particle bed, reducing energy losses during heating and improving overall process efficiency. Proper management of density is crucial to prevent operational issues such as channeling or uneven heating, which could compromise reaction efficiency and product yields. This property is a key consideration in designing reactors that balance material throughput with energy efficiency, making it vital for both laboratory-scale experiments and industrial-scale hydrogen production systems. The density of Cu_2OCl_2 supports scalable reactor designs, ensuring reliable performance in large-scale applications while minimizing operational costs [28].

Importance in the Cu-Cl Cycle

1. **Optimized Reactor Design:** The high density informs optimal fill volume calculations, maximizing reactor capacity and ensuring efficient use of space for high-throughput hydrogen production [28].
2. **Uniform Heat Distribution:** Dense particles promote consistent heat transfer across the reactor bed, improving reaction efficiency and ensuring high yields of CuCl and O_2 [10].
3. **Fluidization Efficiency:** Density supports stable fluidization, reducing energy losses and ensuring smooth particle flow, critical for continuous and reliable operation [25].
4. **Efficient Material Transport:** High density facilitates reliable solid handling, minimizing blockages or flow disruptions, enhancing operational continuity in the reactor system [10].
5. **Process Scalability:** Accurate density data enables scalable reactor designs, ensuring consistent performance in large-scale industrial applications for hydrogen production [8].
6. **Safety Enhancement:** Proper density management prevents reactor overloading, reducing risks of equipment failure or safety hazards, improving the reliability of the thermolysis process [29].

2.2.3. Particle Size:

Cu_2OCl_2 particles, ranging from 50–200 μm , are a key determinant of surface area and heat transfer rates, directly impacting reaction kinetics and solid transport during the thermolysis step [8], [9], [38], [39], [40]. Smaller particle sizes increase the surface area available for heat absorption, accelerating decomposition rates and enhancing reaction efficiency, which is critical for optimizing the Cu-Cl cycle. However, the particle size range must be carefully controlled to balance reaction speed with practical handling considerations, such as fluidization and transport in reactors. This size range ensures efficient particle flow in fluidized beds, preventing issues like agglomeration or uneven flow that could disrupt the process. The particle size also influences the uniformity of heat transfer within the reactor bed, ensuring consistent decomposition across all particles. By optimizing particle size, the thermolysis step achieves faster reaction rates, improved energy efficiency, and reliable material handling, making it a vital factor in both laboratory and industrial-scale applications. This property supports scalable reactor designs and continuous operation, aligning with the cycle's goal of sustainable hydrogen production [25].

Importance in the Cu-Cl Cycle

1. Enhanced Reaction Rates: Smaller particle sizes increase surface area, improving heat transfer and accelerating decomposition, significantly boosting the efficiency of the thermolysis step [25].
2. Efficient Heat Transfer: Optimal particle sizes ensure uniform heating, reducing energy losses and enhancing reaction consistency for high product yields [28].
3. Smooth Material Handling: Controlled particle sizes facilitate fluidization and transport, minimizing blockages and ensuring continuous reactor operation, critical for large-scale systems [10].
4. Process Optimization: Tailored particle sizes balance reaction kinetics and handling efficiency, optimizing the thermolysis step for maximum productivity and reliability [8].
5. Scalability for Industrial Use: Consistent particle size supports scalable reactor designs, ensuring reliable performance in large-scale hydrogen production systems [28].
6. Safety Assurance: Proper particle size management reduces dusting risks, protecting workers and equipment from hazards and maintaining operational safety [29].

2.2.4. Color:

Cu_2OCl_2 exhibits a distinctive greenish-yellow color, serving as a valuable visual indicator for material identification and reaction monitoring during the thermolysis process [24]. This unique color allows operators to verify the presence of the correct material and detect impurities or reaction progress through observable color changes, enhancing quality control. The visual cue is particularly useful in real-time process monitoring, enabling rapid assessment without the need for complex analytical tools, which streamlines operations and reduces costs. The color of Cu_2OCl_2 remains consistent under typical handling conditions, ensuring reliable identification throughout the material's lifecycle in the Cu-Cl cycle. This property supports operational efficiency by minimizing errors in material handling and ensuring that only high-quality Cu_2OCl_2 is processed in the reactor. The ability to monitor reaction progress visually is critical for maintaining consistent decomposition behavior, especially in large-scale systems where rapid detection of anomalies is essential. This characteristic enhances the reliability, safety, and scalability of the thermolysis step in industrial hydrogen production [10].

Importance in the Cu-Cl Cycle

1. Quality Control: The greenish-yellow color enables easy identification, ensuring the correct material is used, preventing processing errors and maintaining process integrity [10].
2. Real-Time Reaction Monitoring: Color changes indicate reaction progress or impurities, allowing operators to adjust conditions promptly, enhancing process control [24].
3. Operational Efficiency: Visual cues reduce the need for complex analytical equipment, minimizing downtime and improving efficiency in large-scale operations [8].

4. Safety Assurance: Color verification prevents the use of contaminated or incorrect materials, reducing the risk of unexpected reactions or safety incidents [29].
5. Process Reliability: Consistent color ensures material integrity, supporting predictable decomposition behavior and reliable cycle performance [10].
6. Cost Efficiency: Simplified monitoring through visual indicators reduces operational costs by minimizing the need for expensive analytical tools [25].

2.3 Thermal Properties

With a specific heat capacity of $\sim 0.45 \text{ J/g}\cdot\text{K}$, thermal conductivity of $\sim 0.48 \text{ W/m}\cdot\text{K}$, and thermal diffusivity of $\sim 0.15 \text{ mm}^2/\text{s}$ at 550°C , Cu_2OCl_2 efficiently absorbs and distributes heat, ensuring uniform decomposition [20], [41], [42], [43]. These properties minimize energy waste, support consistent reaction conditions, and inform reactor heating system design, critical for achieving high yields and scalability in hydrogen production.

2.3.1. Specific Heat Capacity:

Copper oxychloride (Cu_2OCl_2) has a specific heat capacity of approximately $0.45 \text{ J/g}\cdot\text{K}$ at 550°C , a key thermal property that determines the amount of energy required to raise the material's temperature to its decomposition range of $500\text{--}530^\circ\text{C}$ [20]. This relatively low specific heat capacity indicates that Cu_2OCl_2 requires moderate energy input to reach the reaction temperature, making it energy-efficient for the thermolysis step. The specific heat capacity influences the reactor's energy balance, ensuring that heat is effectively utilized to drive the endothermic decomposition without excessive energy waste. This property is critical for designing heating systems that deliver precise and uniform heat to the bed, maintaining consistent reaction conditions across the reactor. Accurate knowledge of the specific heat capacity allows for optimized energy input calculations, reducing operational costs and enhancing process sustainability. In large-scale applications, this property supports the integration of Cu_2OCl_2 with high-temperature heat sources, such as nuclear or solar thermal energy, by minimizing the energy required for preheating. The specific heat capacity also plays a role in preventing thermal gradients within the reactor bed, ensuring uniform decomposition and high product yields, making it a vital factor for both laboratory and industrial-scale hydrogen production [10].

Importance in the Cu-Cl Cycle

1. Energy Balance Optimization: Accurate specific heat capacity data ensures precise energy input calculations, minimizing waste and optimizing the energy balance of the thermolysis step [10].
2. Efficient Heating: The low specific heat capacity reduces the energy needed to reach decomposition temperature, enhancing process efficiency and reducing the energy footprint [8].
3. Reactor Design: This property informs the design of heating systems, ensuring uniform temperature distribution across the reactor bed, critical for consistent reaction performance [28].
4. Cost Efficiency: Optimized energy use lowers operational costs, improving the economic viability of the Cu-Cl cycle for large-scale hydrogen production [10].
5. Process Stability: Consistent specific heat capacity ensures predictable heating behavior, reducing fluctuations in reaction kinetics and enhancing process reliability [20].
6. Safety Assurance: Proper energy management prevents overheating, reducing risks of equipment damage or safety incidents, thereby improving operational safety [29].

2.3.2. Thermal Conductivity:

Cu_2OCl_2 exhibits a thermal conductivity of approximately $0.48 \text{ W/m}\cdot\text{K}$ at 550°C , which governs the rate of heat transfer within the bed during the thermolysis step [43]. This moderate thermal conductivity ensures efficient heat distribution across the particle bed, promoting uniform heating and consistent decomposition rates. Thermal conductivity is critical for preventing localized hot spots or thermal gradients that could lead to incomplete reactions or side reactions, compromising product yields. In fluidized or packed-bed reactors, this property facilitates rapid heat penetration, ensuring that all particles reach the decomposition temperature simultaneously. The thermal conductivity of Cu_2OCl_2 supports the design of efficient

heat transfer systems, minimizing energy losses and enhancing reactor performance. This property is particularly important in large-scale applications, where uniform heating is essential for maintaining high reaction efficiency and scalability. By optimizing heat transfer, Cu_2OCl_2 's thermal conductivity aligns with the Cu-Cl cycle's goal of sustainable hydrogen production, enabling integration with high-temperature heat sources and reducing operational costs. The ability to maintain consistent heat distribution also enhances process reliability, making this property a key factor in industrial reactor design [28].

Importance in the Cu-Cl Cycle

1. **Uniform Heating:** High thermal conductivity ensures even heat distribution, promoting consistent decomposition rates and maximizing product yields [28].
2. **Energy Efficiency:** Efficient heat transfer reduces energy losses, optimizing the use of thermal energy inputs and enhancing process sustainability [10].
3. **Reaction Consistency:** Preventing localized hot spots ensures uniform reaction kinetics, improving the reliability and efficiency of the thermolysis step [8].
4. **Reactor Design:** Thermal conductivity informs the design of heat transfer systems, enhancing reactor performance and supporting scalability for industrial applications [28].
5. **Cost Savings:** Reduced energy waste lowers operational costs, improving the economic feasibility of the Cu-Cl cycle for hydrogen production [10].
6. **Safety Enhancement:** Uniform heating minimizes risks of thermal runaway or equipment damage, enhancing process safety and operational reliability [29].

2.3.3. Thermal Diffusivity:

Cu_2OCl_2 has a thermal diffusivity of approximately $0.15 \text{ mm}^2/\text{s}$ at 550°C , calculated from its thermal conductivity, density, and specific heat capacity, which influences the speed and uniformity of heat penetration within the particle bed [24], [43]. This property determines how quickly heat spreads through the solid material, ensuring that all particles reach the decomposition temperature efficiently. High thermal diffusivity is critical for achieving uniform heating in fluidized or packed-bed reactors, preventing temperature gradients that could lead to inconsistent reaction rates or incomplete decomposition. The thermal diffusivity of Cu_2OCl_2 supports rapid heat transfer, reducing the time required to initiate and sustain the decomposition reaction, thereby improving process efficiency. This property is essential for designing reactors that maintain consistent temperature profiles, particularly in large-scale systems where heat distribution challenges are more pronounced. By facilitating uniform heating, thermal diffusivity enhances reaction reliability, minimizes energy losses, and supports integration with high-temperature heat sources like nuclear or solar thermal energy. This characteristic is vital for ensuring scalability, cost-effectiveness, and sustainability in industrial hydrogen production, making it a key consideration in the thermolysis step [10].

Importance in the Cu-Cl Cycle

1. **Heating Uniformity:** High thermal diffusivity ensures rapid and even heat distribution, enhancing reaction consistency and maximizing product yields [10].
2. **Process Efficiency:** Faster heat penetration reduces energy requirements, optimizing the thermolysis step and improving overall energy efficiency [8].
3. **Reactor Performance:** Supports efficient reactor designs by minimizing temperature gradients, enhancing scalability and operational reliability [28].
4. **Reaction Stability:** Uniform heating prevents kinetic variations, ensuring consistent decomposition behavior and reliable process performance [25].
5. **Cost Efficiency:** Reduced energy needs lower operational costs, enhancing the economic viability of the Cu-Cl cycle for large-scale applications [10].
6. **Safety Assurance:** Even heat distribution minimizes risks of overheating or thermal stress, improving reactor safety and protecting equipment [29].

2.4 Mechanical Properties

Cu_2OCl_2 's bulk density of $\sim 2.1 \text{ g/cm}^3$ and Mohs hardness of ~ 2.5 indicate efficient packing but susceptibility to attrition, requiring careful handling to prevent dusting [44], [45]. These properties optimize reactor loading and fluidization while necessitating robust containment systems, ensuring material integrity, worker safety, and cost-effective operation.

2.4.1. Bulk Density:

Cu_2OCl_2 has a bulk density of 2.1 g/cm^3 , a critical property that affects solid handling, reactor loading efficiency, and material flow dynamics during the thermolysis step [45]. This bulk density, lower than the material's true density, allows for efficient packing in fluidized or packed-bed reactors, optimizing space utilization and ensuring smooth particle movement. The bulk density determines the volume of material that can be loaded into the reactor, directly influencing process throughput and energy efficiency. A well-managed bulk density minimizes energy requirements for material transport and supports stable fluidization, preventing issues like channeling or uneven flow. This property is essential for designing reactors that balance material handling with operational efficiency, making it a key consideration for both laboratory and industrial-scale hydrogen production. The bulk density of Cu_2OCl_2 supports scalable reactor designs, ensuring consistent performance in large-scale applications while reducing operational disruptions and costs. This characteristic enhances the reliability and scalability of the Cu-Cl cycle, aligning with the goal of sustainable hydrogen production [28].

Importance in the Cu-Cl Cycle

1. Efficient Reactor Loading: The bulk density ensures optimal reactor capacity utilization, maximizing throughput and enhancing process efficiency in hydrogen production [28].
2. Smooth Material Handling: Lower bulk density facilitates consistent material flow, reducing blockages and ensuring continuous operation in reactors, critical for large-scale systems [10].
3. Energy Efficiency: Efficient packing minimizes energy waste in material transport and heating, optimizing the energy balance of the thermolysis step [8].
4. Scalability for Industrial Applications: Bulk density data supports large-scale reactor designs, ensuring consistent performance in industrial hydrogen production [28].
5. Cost Savings: Reduced handling issues lower maintenance and operational costs, improving the economic viability of the Cu-Cl cycle [10].
6. Safety Enhancement: Proper bulk density management prevents overloading, reducing risks of equipment failure or safety hazards, improving operational reliability [29].

2.4.2. Hardness:

Cu_2OCl_2 has a Mohs hardness of 2.5, indicating a relatively soft material that is susceptible to attrition and dusting during handling in the thermolysis step [45]. This low hardness requires careful design of handling systems to minimize particle breakdown, which could lead to material loss, dust generation, or equipment fouling. The soft nature of Cu_2OCl_2 necessitates robust containment systems to prevent dust inhalation by workers, which could pose health risks, and to protect reactor components from dust accumulation. Effective management of hardness ensures material integrity, reduces operational losses, and enhances worker safety, making it a critical consideration for process design. The low hardness also influences the choice of handling equipment, favoring systems that minimize mechanical stress on particles. This property is particularly important in large-scale applications, where material loss or dust-related issues could significantly impact operational efficiency and costs. By addressing hardness-related challenges, the thermolysis step achieves reliable material handling, consistent decomposition behavior, and enhanced scalability for industrial hydrogen production [29].

Importance in the Cu-Cl Cycle

1. Minimized Material Loss: Controlled handling of soft Cu_2OCl_2 reduces attrition, preserving material for efficient decomposition and maximizing reaction yields [29].

2. Worker Safety: Low hardness requires dust containment to protect workers from inhalation risks, ensuring a safe working environment in large-scale operations [29].
3. Equipment Protection: Reduced dusting prevents fouling or clogging of reactor components, extending equipment lifespan and minimizing maintenance costs [10].
4. Process Efficiency: Minimized material loss ensures maximum reactant availability, optimizing the thermolysis step's productivity and reliability [8].
5. Cost Efficiency: Lower maintenance and material replacement costs due to reduced attrition improve the economic feasibility of the cycle [10].
6. Operational Stability: Controlled handling maintains consistent material properties, supporting reliable decomposition behavior and process performance [28].

4. Conclusion

This paper comprehensively evaluated the chemical, physical, thermal, mechanical, thermodynamic and kinetic properties of copper oxychloride (Cu_2OCl_2) and their critical role in the thermolysis step of the Cu–Cl thermochemical cycle for hydrogen production. The analysis highlights how Cu_2OCl_2 's well-defined thermal decomposition, phase stability, high purity, and low reactivity with reactor materials contribute to efficient, predictable, and scalable hydrogen generation. Properties such as specific heat capacity, thermal conductivity, density, particle size, and activation energy directly influence reactor design, energy balance, and operational safety. The findings confirm that the successful performance of the thermolysis step—and by extension, the entire Cu–Cl cycle—relies heavily on selecting and handling materials with well-characterized and favorable properties. By providing a material-focused assessment, this paper supports the development of optimized thermochemical systems and offers guidance for future experimental and industrial applications of the Cu–Cl cycle in sustainable hydrogen production.

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