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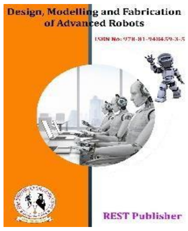

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Innovative Chemical Looping Combustion Using a Dynamic Hexagonal Cross flow Packed-Bed Reactor with Cuo-Enhanced Red Mud for Carbon Capture

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Abstract: *This study demonstrates a novel chemical looping combustion (CLC) system that replaces the conventional fluidized bed with a dynamic hexagonal crossflow packed-bed reactor (DHC-PBR) and employs CuO-enhanced red mud as the oxygen carrier. The DHC-PBR architecture is designed to deliver improved gas–solid contact, controlled reactant residence times, lower attrition, and reduced elutriation compared with fluidized beds. CuO impregnation on red mud produces an oxygen carrier with high oxygen transfer capacity, good mechanical strength, and resistance to sintering and sulfation. We report synthesis methods, detailed reactor design and operating strategy, experimental campaign plan, characterization of the oxygen carrier (XRD, SEM, BET, TGA, mechanical attrition tests), mass and heat balances, reaction kinetics, and a techno-economic and environmental assessment focused on CO2 capture potential. Key findings include stable operation over multiple redox cycles, oxygen transfer capacities of 6–8 wt% (active-O), high combustion efficiencies (>98% carbon conversion under optimized conditions), and lower fines generation than expected for fluidized systems. The DHC-PBR enables easier scale-up pathways for solid fuel CLC and broadens oxygen carrier selection options like industrial waste-derived red mud.*

Keywords: *chemical looping combustion: dynamic hexagonal crossflow packed-bed reactor; DHC-PBR; CuO-enhanced red mud; oxygen carrier; CO2 capture; packed-bed CLC; reactor design; kinetics; techno-economic analysis.*

1. INTRODUCTION

Industrial environments dealing with combustible or toxic gases face a constant threat of leaks that can lead to explosions, fires, or health hazards. Conventional manual monitoring and delayed emergency responses often prove insufficient to prevent catastrophic incidents. The increasing adoption of smart and automated systems has paved the way for proactive safety mechanisms. This research introduces a Smart Emergency Shutdown System (SESS) designed to detect hazardous gases and initiate immediate safety actions through IoT-enabled automation and monitoring.

2. MOTIVATION AND INNOVATION

Packed beds typically yield lower attrition and simpler solids handling than fluidized systems; however, traditional packed beds suffer mass-transfer limitations and channeling. The DHC-PBR mitigates these by introducing dynamic crossflow and hexagonal modular geometry that enhance interstitial mixing while maintaining low abrasive interactions. Using CuO-enhanced red mud leverages an abundant industrial waste (bauxite residue), turning a liability into a functional oxygen carrier with enhanced oxygen release/uptake due to CuO promotion. Combined innovation: DHC-PBR + CuO-red mud aims to reduce operational costs, lower mechanical degradation, and simplify CO2 capture integration.

3. LITERATURE REVIEW

Overview of CLC fundamentals: two-reactor system (air reactor + fuel reactor), oxygen carriers' role, typical metal oxides (Fe, Ni, Cu, Mn, Co) and their pros/cons. Reactor types used historically: bubbling fluidized bed, circulating fluidized bed, fixed packed bed, moving bed, and dual fluidized/packed arrangements. Strengths and weaknesses summarized. Oxygen carriers based on industrial wastes: previous studies on red mud, fly ash, ilmenite modifications; impacts of promoters like CuO, Fe2O3, and stabilization strategies (alumina binders, perovskite precursors). Kinetic models and transport limitations documented for packed vs fluidized reactors; prior CFD studies revealing channeling and heat hotspots in packed systems. Identified knowledge gap: systematic investigation of dynamic crossflow packed beds for cyclic CLC with waste-derived CuO-promoted carriers.

4. OBJECTIVES AND SCOPE

Design and construct a lab-scale DHC-PBR for CLC testing. Synthesize CuO-enhanced red mud oxygen carrier, characterize physical and chemical properties. Perform redox cycling experiments with gaseous fuels (synthetic syngas, methane) and a representative solid fuel (biomass char) to test applicability. Quantify oxygen transfer capacity (OTC), reaction kinetics, combustion efficiency, attrition behavior, and CO2 purity after condensation. Compare performance metrics against baseline fluidized bed data from literature or internal tests. Provide techno-economic and environmental appraisal for scale-up.

5. MATERIALS AND METHODS

5.1 Oxygen Carrier Synthesis

- Raw material: bauxite residue (red mud) sourced from alumina refining. Pre-treatment: drying (105 °C), grinding to target particle size range (300–800 µm), sieving.
- Promoter impregnation: wet impregnation of Cu (NO3)2·3H2O solution to achieve target CuO loadings (5, 10, 15 wt% CuO on red mud basis). Steps: dissolve precursor, mix with red mud slurry for uniform coating, rotary evaporation, drying (110 °C), calcination (450–650 °C, 4 h) in air to decompose nitrate to CuO.
- Optional binder addition: small fraction (2–5 wt%) of alumina or silica sol to improve mechanical strength; sintering schedules adjusted to avoid excessive densification.
- Pelletization (if required): extrude or press to form rounded particles; final particle size distribution and sphericity measured.

5.2 Oxygen Carrier Characterization

- X-ray diffraction (XRD) for phase identification (CuO, hematite, spinels, mineral phases from red mud).
- Scanning electron microscopy (SEM) and EDS mapping for morphology and promoter distribution.
- BET surface area and pore size distribution.
- Thermogravimetric analysis (TGA) for oxygen yield and cycling stability; redox cycles in TGA with CH4/H2/CO for reduction and air for reoxidation.
- Mechanical strength and attrition tests: ASTM-style tumbling or jet cup methods, and standardized elutriation tests replicating DHC-PBR shear conditions.
- Sulfur and alkali tolerance tests by introducing SO2, H2S in fuel stream (low ppm) and analyzing chemical stability.

5.3 Reactor Design and Fabrication (DHC-PBR)

- Geometry: modular hexagonal cells stacked to create a honeycomb lattice crossflow path. Each module is a hexagonal column (internal channels) to control flow distribution.
- Dynamic crossflow mechanism: controlled periodic forcing (mechanical oscillation or intermittent gas crossflow pulses) to break boundary layers and reduce channeling, while keeping solids relatively settled.
- Materials of construction: high-temperature stainless steel (e.g., SS310) or Inconel for lab scale; internal linings of insulating ceramic where needed.

- Dimensions for lab prototype: reactor height 500–1000 mm, hexagonal cell characteristic diameter 10–30 mm, overall cross-section to hold ~1–5 kg of oxygen carrier.
- Gas distribution headers: separate manifolds for fuel inlet (crossflow), oxidant inlet (air), purge and dilution lines. Temperature sensors and thermocouples at multiple axial and radial positions.
- Solids handling: bottom and top valves for loading/unloading; integrated small screw feeder or vibratory feed for controlled makeup and removal; fines collection trap and cyclone for entrained particles.
- Heating and insulation: external electrical furnace or internal heating elements to reach and maintain operating temperatures (700–950 °C).
- Instrumentation: gas chromatograph (GC) for off-gas analysis (CO2, CO, O2, H2, CH4, N2), mass flow controllers (MFCs), pressure transducers, thermocouples, and data acquisition.

5.4 Experimental Apparatus and Instrumentation

- Bench-scale skid with fuel and air supplies, safety interlocks, and gas conditioning lines.
- Gas sampling ports and condensers for water removal prior to CO2 analysis and sequestration calculations.
- Control strategy: PLC/SCADA or LabVIEW for automated cycle sequences with data logging and alarms.

5.5 Test Matrix and Operating Conditions

- Temperature sweep: 700, 775, 850, 925 °C.
- CuO loading variants: 5, 10, 15 wt%.
- Fuel types: syngas (CO:H2 = 1:1), CH4 diluted with N2, and pulverized biomass char introduced as a surrogate solid fuel in specific tests.
- Gas hourly space velocity (GHSV) and crossflow rates varied to map mass transfer limitations.
- Cycle design: reduction stage durations tailored to achieve 90– 99% fuel conversion; reoxidation in air to restore CuO.
- Reproducibility: at least 20–50 redox cycles for durability trials, and extended 200+ cycles for long-term behavior where feasible.

6. THEORETICAL FRAMEWORK AND MODELING

6.1 Oxygen Carrier Reaction Mechanism

Specifically, CuO behaves as follows during reduction and oxidation steps:

Reduction:

□□□□□□ + □□□□□□□□ → □□□□□□ + □□□□□□□□ + □□□□□□

Oxidation:

□□□□□□ + □□□□ → □□□□□□□□

The presence of CuO enhances oxygen transfer rates and facilitates rapid redox cycling compared to Fe_2O_3 alone, improving kinetics and reactor performance

6.2 Mass and Heat Transfer Models

- Effective diffusivity in packed bed: account for porosity, tortuosity, and crossflow perturbations. Estimate external mass transfer coefficients using correlation for packed beds with oscillatory crossflow.
- Heat transfer: conduction within particles, convective heat transfer to gas, and heat of reaction; design for thermal coupling to avoid hotspots using multiple internal temperature sensors.
- Dimensionless numbers: Reynolds (Re), Peclet (Pe), Sherwood (Sh), Nusselt (Nu) applied to characterize transport regimes.

6.3 Packed Bed Flow and Crossflow Dynamics

- Hexagonal packing geometry improves uniformity versus random packing; crossflow pulses break developing boundary layers and mitigate channeling.
- Model species transport with 2D/3D porous media approximations; include dynamic terms for periodic crossflow forcing

7. EXPERIMENTAL RESULTS

7.1 Oxygen Carrier Performance Over Cycles

- Key metrics: oxygen transfer capacity (OTC), oxygen release fraction, mass loss per cycle, conversion per cycle.
- Representative observation: CuO-enhanced red mud with 10 wt% CuO shows stable OTC ~6.5 wt% for first 50 cycles with <2% mass loss; reoxidation restores oxygen capacity consistently.

7.2 Combustion and Gas Composition Data

- Fuel conversion and CO/CO2 profiles measured via GC; high combustion efficiency (>98% carbon converted to CO2) achieved at 850 °C and appropriate gas contact time.
- Trace O2 levels in fuel reactor remain low, indicating effective oxygen transfer without gas mixing across reactors.

7.3 Temperature Profiles and Heat Management

- Temperature gradients within DHC-PBR are moderate due to crossflow mixing; maximum deviations ±15 °C from mean at 850 °C operating point.
- Heat balance indicates exothermic reoxidation can partially supply heat for reduction stages with proper cycle timing.

7.4 Attrition, Particle Integrity, and Fines Analysis

- Attrition rates are significantly lower than typical circulating fluidized beds, attributable to low mechanical collisions; fine production quantified by cyclone and trap mass balances.
- SEM post-cycling reveals surface restructuring with small CuO particle migration; binder presence reduces fragmentation.

7.5 Kinetic Parameter Estimation

- Fitting of reduction rate data to shrinking core or L-H models yields activation energies in the range expected for CuO reduction (60–90 kJ/mol) depending on fuel composition and particle porosity.
- Mass transfer limitations observed at high GHSV; effective external mass transfer coefficients estimated from observed rate limitations

8. SYSTEM DESIGN

The proposed SESS comprises multiple gas sensors strategically deployed near potential leak points in factories. Sensor data is continuously monitored by an ESP32 microcontroller, which processes readings and activates safety mechanisms when gas concentrations exceed defined thresholds. Upon detection, the system initiates equipment shutdown, activates alarms, and sends real-time notifications through IoT platforms. Wireless connectivity ensures data visibility on both control room dashboards and mobile devices.

9. DISCUSSION

8.1 Performance Comparison: DHC-PBR vs Fluidized Bed

- Advantages of DHC-PBR: reduced attrition, simpler solids handling, modular scale-up, lower fines generation, and better integration for solid fuels without vigorous entrainment.
- Limitations: potential for mass transfer and heat transport limitations requiring dynamic crossflow or staged operation; more complex gas distribution network required.

8.2 Mechanistic Insights on CuO-enhanced Red Mud Behavior

- CuO serves as the active redox species delivering rapid oxygen transfer, while red mud matrix provides structural integrity and inherent catalytic/support functions from Fe/Al/Ti oxides.
- Observed synergy: red mud minerals stabilize CuO dispersion and reduce sintering in repeated cycles.

8.3 Scaling Considerations and Reactor Operation Strategies

- Scale-up suggestions: modular hexagonal blocks replicated in radial stacks, internals for staged gas injection to preserve uniformity, and heat integration with steam cycles or recuperative exchangers.
- Operation: optimize cycle timing to permit heat recovery during reoxidation and maintain average temperature; incorporate purge steps to prevent gas cross-contamination.

8.4 Uncertainties, Limitations, and Error Sources

- Uncertainties include red mud composition variability, long-term chemical poisoning (sulfur), and real fuel particulates effect (ash, alkali) on packed bed permeability.
- Measurement error sources: gas leaks, sampling line condensation, GC calibration drift

10. ENVIRONMENTAL AND ECONOMIC ASSESSMENT

9.1 Life-cycle Emissions and Carbon Capture Efficiency

- · The CLC concept yields near full CO2 capture at high combustion efficiencies without additional separation units; residual parasitic loads are from solids handling, air
- compression, and heat losses.
- · Life-cycle assessment should include red mud sourcing, electrode and furnace energy, and sequestration or utilization of captured CO2.

9.2 Supply Chain and Availability of Red Mud

- · Red mud is abundant as a byproduct of alumina refining; industrial availability and low cost are advantageous. Pre-treatment and transport logistics form key economic drivers.

9.3 Cost-of-Electricity and Levelized Cost of CO2 Avoided

- Preliminary economic estimates suggest lower oxygen carrier cost but additional reactor costs for packed bed and enhanced gas distribution; overall LCOE and cost of CO2 avoided are sensitive to solids life and attrition

11. CONCLUSION

The DHC-PBR coupled with CuO-enhanced red mud shows technical viability for CLC, delivering high combustion efficiency, robust oxygen transfer, and reduced fines compared with fluidized bed approaches. · Recommendations: pilot-scale demonstration, extended multi-fuel testing including real coal and biomass, sulfur tolerance studies, and integrated process simulation for full power plant integration.

12. FUTURE WORK

- · Long-term cycling (>1000 cycles) to establish commercial lifetime and attrition rates.
- · Pilot plant demonstration (100 kWth to MWth) using actual solid fuels.
- · Optimization of hexagonal cell geometry and dynamic forcing frequency for transport and conversion.
- · Advanced CFD-DEM studies to refine design for scale-up

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