**SRI VENKATESWARA INTERNSHIP PROGRAM**
**FOR RESEARCH IN ACADEMICS**
**(SRI-VIPRA)**

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# Project Report of 2025: SVP-2532

## "Efficient one-pot capture and conversion of $CO_2$ to methanol using Ionic liquids"

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## SRIVIPRA PROJECT (SVP-2532)

**Title:** Efficient one-pot capture and conversion of $CO_2$ to methanol using Ionic liquids

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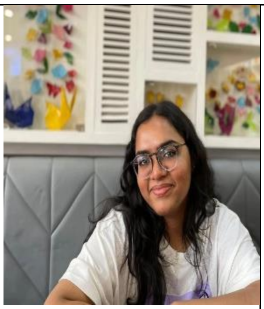
| 3 |  | Gauri Jha | 1324014 | B.Sc. (hons) Biological Sciences | Gauri |
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# Certificate of Originality

This is to certify that the students from Sri Venkateswara College have participated in the summer project SVP-2532 titled "Efficient one-pot capture and conversion of $CO_2$ to methanol using Ionic liquids". The participants have carried out the research project work under my guidance and supervision from 1st July 2025 to 15th September 2025. The work carried out is original and carried out in an online/offline/hybrid mode.

Meena

**Signature of Mentor**

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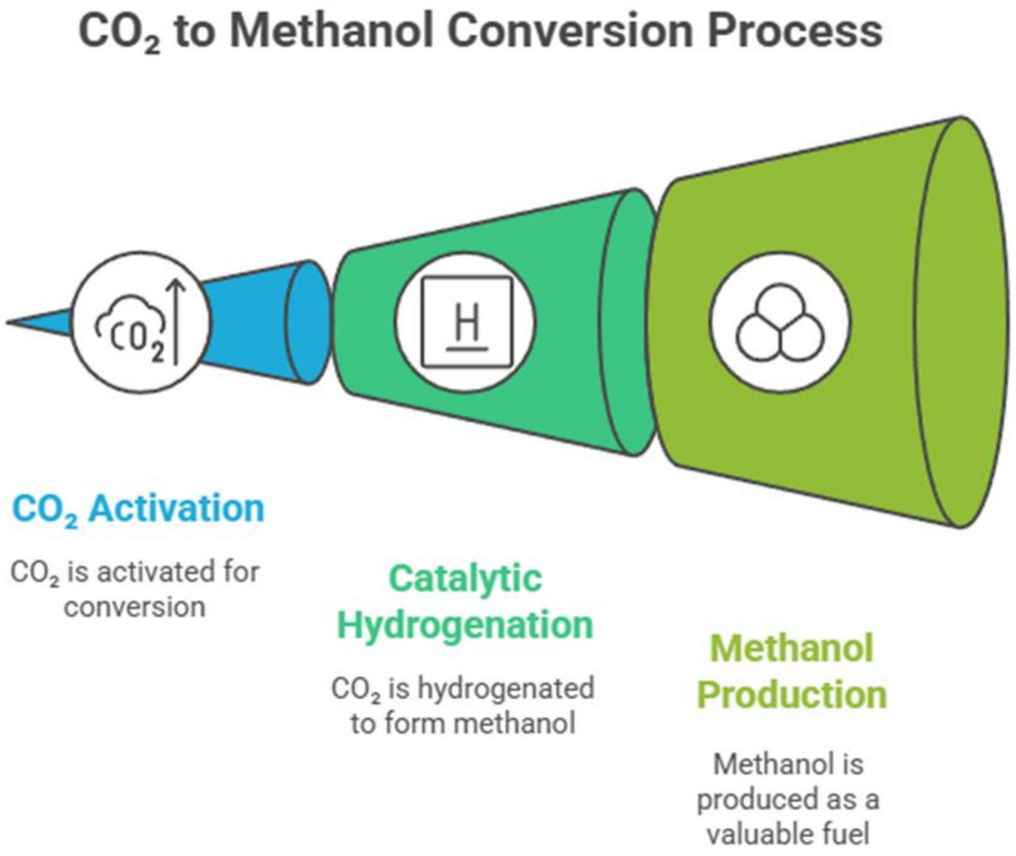
# Summary of the Project

The report discusses an innovative method for carbon capture and utilization that combines the absorption and conversion of $CO_2$ into methanol using ionic liquids (ILs). Unlike conventional amine-based systems, ILs offer high stability, tunability, and efficiency with lower environmental impact. The study highlights recent advances in IL design, including porous, amino-functionalized, and dual-functionalized systems, which enhance both $CO_2$ capture and reactivity. It also reviews catalytic hydrogenation processes using Cu- and $CeO_2$-based catalysts for methanol synthesis. Integrating these into a one-pot IL–catalyst system minimizes energy use and simplifies operation, supporting circular carbon management. The report concludes by emphasizing the need for improved IL–catalyst compatibility, system stability, and scalable reactor designs for sustainable, low-carbon methanol production.

# One-Pot Capture and Conversion of $CO_2$ to Methanol Using Ionic Liquids: A Pathway to Circular Carbon Management

*Graphical Abstract*



## *1. Introduction*

The urgent need to mitigate climate change has accelerated global efforts toward developing carbon-neutral technologies, with carbon dioxide ($CO_2$) management occupying center stage in scientific discourse. Despite decades of research and policy intervention, $CO_2$ emissions—largely generated from fossil fuel combustion and industrial expansion—remain at record highs, pushing atmospheric levels beyond safe thresholds and intensifying the call for innovative solutions that balance sustainability with industrial feasibility (Bisht et al., 2023; Pandey et al., 2025). This imperative has heightened interest in Carbon Capture, Utilization, and Storage (CCUS) strategies, which seek not only to remove $CO_2$ from emission sources but also to valorize it as a feedstock for valuable chemicals and fuels (Pandey et al., 2025).

Conventional $CO_2$ capture technologies, most notably those employing aqueous amine solvents, have underpinned much of the progress in carbon management to date. However, these methods are hindered by several well-documented drawbacks: high energy input for solvent regeneration, volatility and corrosivity, environmental concerns related to degradation by-products, and rising operational costs (Bisht et al., 2023; Pandey et al., 2025). As a result, recent research has pivoted toward discovering and designing materials that offer high capture performance coupled with easy regeneration, stability, and reduced lifecycle impacts (Bisht et al., 2023; Alguacil & Robla, 2024).

Ionic liquids (ILs) have rapidly emerged as promising alternatives to traditional sorbents, owing to their unique blend of properties: negligible vapor pressure, high thermal and chemical stability, customizable structure, and notably, exceptional $CO_2$ solubility (Bisht et al., 2023; Alguacil & Robla, 2024). This tunability means that ILs can be precisely engineered to optimize both $CO_2$ uptake and subsequent reactivity, supporting not only physical absorption but also providing a versatile reaction medium for catalytic transformations. Recent advances have shown that ILs can outperform classical aqueous amine systems in selectivity, cyclic stability, and energy efficiency under many scenarios of $CO_2$ capture (Alguacil & Robla, 2024; Pereira et al., 2025).

The true potential of ILs, however, lies in their ability to integrate $CO_2$ capture with direct chemical transformation in a single, streamlined process—sometimes referred to as "one-pot" or integrated capture and conversion (Pereira et al., 2025; Pandey et al., 2025). This approach eliminates intermediate steps like $CO_2$ desorption and recompression, instead activating captured $CO_2$ in-situ for reaction with hydrogen or other substrates to yield value-added products such as methanol. Such synergy not only optimizes energy usage and operational footprints but also aligns with goals of process intensification and circular economy (Pereira et al., 2025).

Recent studies underscore the practical viability of this approach. Notably, systems coupling ILs with catalysts such as Cu/MgO or supported polymer-metal hybrids enable the direct hydrogenation of $CO_2$ to methanol under relatively mild conditions, consistently achieving high selectivity and throughput (Pandey et al., 2025). Novel advances in IL design—including bifunctional structures tailored for both $CO_2$ binding and activation—further expand the chemical space accessible for conversion chemistries, while advances in immobilized and polymer-supported IL phases have made strides in stability, recyclability, and resistance to impurities from real-world gas streams (Alguacil & Robla, 2024; Ni et al., 2025). For instance, newly reported metal-ionic polymer composites have been shown to maintain robust $CO_2$ uptake and catalytic performance even in the presence of challenging contaminants, marking encouraging progress toward industrial deployment (Ni et al., 2025).

Taken together, recent developments in the design and application of ionic liquids underscore an emerging paradigm in carbon management. By uniting their strong $CO_2$ sorption capacity with tailored catalytic functionalities, it is now possible to envision integrated one-pot systems that simultaneously capture and convert $CO_2$ into valuable products such as methanol. This dual capability not only enhances process efficiency and energy utilization but also aligns with broader goals of circular economy and sustainable chemical manufacturing. Ongoing innovations in catalyst–IL hybrid systems, polymer-supported phases, and bifunctional IL structures continue to address key challenges of stability, scalability, and tolerance to real-world gas streams. Collectively, these advances highlight both the promise and the remaining hurdles on the path toward industrial implementation of IL-based $CO_2$ valorization technologies.

This review critically examines (i) IL design strategies for $CO_2$ capture, (ii) advances in catalytic hydrogenation to methanol, and (iii) the integration of the two into one-pot IL–catalyst systems that embody the future of circular carbon technologies.

## *2. Ionic Liquid Strategies for $CO_2$ Capture*

The modularity of ILs—the ability to finely tune cation–anion combinations and introduce functional groups—confers significant advantages over conventional solvents. Not only can ILs achieve high $CO_2$ uptake, but they also provide a versatile medium for further catalytic conversion of the captured $CO_2$. Recent reports (Table 1) show that IL-based systems can outperform aqueous amines in terms of selectivity, cyclic stability, and energy efficiency across many operating conditions (Alguacil & Robla, 2024; Pereira et al., 2025). Crucially, the true potential of ILs lies in their capacity to merge capture and utilization into an integrated process. Instead of relying on a multistep cycle of absorption, desorption, compression, and reaction, ILs enable "one-pot" schemes where captured $CO_2$ can be activated in situ for direct transformation into fuels or chemicals such as methanol (Pereira et al., 2025; Pandey et al., 2025). Such integration exemplifies process intensification, reducing energy penalties and simplifying operational footprints while advancing toward circular, low-carbon chemical manufacturing.

Several studies illustrate how ILs can be tailored for this dual function. Avila et al. (2021) demonstrated that porous ionic liquids (PoILs), created by combining phosphonium ILs with ZIF-8 frameworks, enable both chemical binding of $CO_2$ via ylide formation and physical adsorption within the porous scaffold. The resulting composites achieved uptake capacities up to 1.5 mmol $g^{-1}$ at low pressures, underscoring the potential of hybrid IL–framework systems for mild-condition capture. Complementary to this, Huang et al. (2018) developed an amino-functionalized IL, [TETAH][Lys], in a biphasic ethanol–water solvent system that facilitated phase separation of absorption products. This design not only improved cycling efficiency but also highlighted how solvent engineering can overcome viscosity and regeneration barriers common to ILs. Wu et al. (2019) extended the design space by introducing dual-functionalized ILs where both the cation and the heteroanion actively participated in $CO_2$ binding. Their protic IL [DETAH][Im] achieved capacities surpassing conventional amine systems through cooperative binding and proton shuttling, with Tiwari et al. (2022) later confirming the robustness of such systems under repeated cycling. Together, these strategies—functionalized protic ILs, biphasic solvents, and porous IL hybrids—outline a diverse design toolkit for optimizing capture and tailoring downstream reactivity.

Table 1. Ionic Liquid Strategies for $CO_2$ Capture

| **Study / Approach** | **IL System** | **Strategy / Design Feature** | **Key Mechanism** | **$CO_2$ Uptake / Performance** | **Key Insights** |
|---|---|---|---|---|---|
| Avila et al. (2021) | Phosphonium IL + ZIF-8 → Porous IL (PoIL) | Hybrid porous scaffold | Chemical binding via ylide formation + physical adsorption in pores | Up to **1.5 mmol g$^{-1}$** at low pressure | Illustrates hybrid IL–framework synergy under mild conditions |
| Huang et al. (2018) | [TETAH][Lys] in biphasic ethanol–water | Biphasic solvent system | Phase separation of absorption products | Improved cycling efficiency | Overcomes viscosity and regeneration barriers |
| Wu et al. (2019) | [DETAH][Im] (dual-functionalized protic IL) | Both cation + heteroanion active | Cooperative binding, proton shuttling | Higher than conventional amines | Demonstrated robustness under cycling (Tiwari et al., 2022) |

| | | | | | |
|---|---|---|---|---|---|
| General Advances | Functionalized protic ILs, biphasic solvents, porous IL hybrids | Tailored IL design | Integrated capture + activation | High selectivity, stability, and reduced regeneration energy | Outperform aqueous amines in efficiency and cyclic stability |

### *3. Catalytic Hydrogenation of $CO_2$ to Methanol*

The natural next step is linking these advances in capture media with catalytic hydrogenation routes for methanol synthesis, one of the most intensively studied and industrially relevant $CO_2$ utilization pathways. Methanol is a platform chemical with applications spanning fuels, solvents, and polymer precursors, as well as an emerging hydrogen carrier for renewable energy systems. The hydrogenation of $CO_2$ to methanol, however, remains both thermodynamically and kinetically challenging, demanding optimized catalysts and carefully engineered reactors.

Historically, methanol has been produced via syngas hydrogenation ($CO/CO_2/H_2$) over $Cu/ZnO/Al_2O_3$ catalysts in fixed-bed reactors. Industrial processes such as those developed by ICI and Lurgi operate under conditions of 220–270 °C and 5–10 MPa, where thermodynamics favor high conversions at low temperatures and elevated pressures (Yusuf & Almomani, 2023). However, equilibrium limitations necessitate recycling loops and heat management remains a central engineering challenge due to the exothermicity of the reaction ($\Delta H = -87$ kJ/mol). These realities, alongside process simulations and industrial experience, confirm that catalyst design alone cannot guarantee efficiency; reactor engineering and operational strategies are equally decisive.

Slurry-phase processes have been investigated as alternatives to overcome heat and mass transfer limitations inherent to fixed beds. Slurry bubble column reactors (SBCRs), in which gases are dispersed through a liquid phase containing suspended catalysts, enable isothermal operation, high dispersion, and improved control over exothermicity. Schühle et al. (2021) reported stable performance of $In_2O_3/ZrO_2$ catalysts in slurry media, demonstrating how solvent and carrier choices influence transport and reaction dynamics. Building on this, Pandey et al. (2025) showed that CuMgCe catalysts in slurry systems benefit from synergistic interactions between methanol and catalyst interfaces, where methanol itself promotes formate stabilization and $CO_2$ activation. These findings illustrate that slurry reactors are not only intensification tools but also environments where solvent–catalyst–feed interactions actively shape mechanistic pathways.

At the mechanistic level, progress has been made in elucidating the active sites responsible for $CO_2$ activation. Zhu et al. (2020) demonstrated that ceria supports stabilize oxygen vacancies and enhance the formate pathway, which has become widely recognized as the dominant route under $CO_2$-rich feeds. Such defect engineering represents a broader trend in catalyst development, where supports like $CeO_2$ and $ZrO_2$ function not as inert carriers but as active participants that modulate spillover, intermediate stabilization, and hydrogen activation. Yet, despite these innovations, stability challenges remain. Walter et al. (2024) identified sintering of Cu nanoparticles as the primary deactivation mode in liquid-phase methanol synthesis, with liquid environments exacerbating structural collapse. Mitigation strategies—anchoring Cu with stabilizing supports, introducing dopants, and engineering solvent systems—are therefore indispensable for sustainable operation. Summary of the recent literature is shown in Table 2.

Table 2. Catalytic Hydrogenation of $CO_2$ to Methanol

| **Study / Catalyst** | **Reactor / Medium** | **Mechanism / Active Feature** | **Operating Insights** | **Key Challenges / Findings** |
|---|---|---|---|---|
| Industrial (ICI, Lurgi) | Fixed-bed ($Cu/ZnO/Al_2O_3$) | $CO_2$ hydrogenation via formate pathway | 220–270 °C, 5–10 MPa | Equilibrium limits, requires recycle loops, heat management ($\Delta H = –87$ kJ/mol) |
| Schühle et al. (2021) | $In_2O_3/ZrO_2$ in slurry bubble column reactor (SBCR) | Solvent–catalyst interactions improve dispersion | Isothermal operation, better exothermicity control | Demonstrates potential of slurry systems |
| Pandey et al. (2025) | CuMgCe catalysts in slurry media | Methanol stabilizes formate intermediates | Methanol promotes $CO_2$ activation | Synergistic solvent–catalyst effects |
| Zhu et al. (2020) | $CeO_2$-supported catalysts | Oxygen vacancy stabilization | Enhances formate pathway | Defect engineering critical for activation |
| Walter et al. (2024) | Cu nanoparticles in liquid phase | Active Cu sites prone to sintering | Liquid media accelerate collapse | Mitigation via dopants, supports, and solvent engineering |

## *4. One-Pot Integration: ILs as Capture and Reaction Media*

Viewed together, the advances in IL design for $CO_2$ capture and the innovations in catalytic hydrogenation converge on a common vision: integrated systems that simultaneously capture $CO_2$ and convert it into methanol under mild, energy-efficient conditions. ILs, with their tunable solvation environments and ability to stabilize reactive intermediates, are uniquely positioned to serve as both capture agents and reaction media. Catalysts, whether based on Cu/ZnO, $CeO_2$-supported systems, or novel bifunctional materials, provide the necessary activity and selectivity for methanol production. By merging these components, one can imagine one-pot processes where $CO_2$ is absorbed into IL matrices, activated at bifunctional interfaces, and hydrogenated to methanol without the need for desorption or recompression.

Such a paradigm embodies the principles of process intensification and circular economy. It reduces operational energy penalties, minimizes solvent and catalyst losses, and opens the door to modular, distributed methanol production units tailored to localized $CO_2$ sources. Challenges remain, particularly in addressing long-term IL stability, catalyst sintering in liquid environments, and tolerance to real-world flue gas impurities. Yet, ongoing innovations in bifunctional ILs, polymer-supported IL phases, and vacancy-rich catalyst systems continue to close these gaps (Alguacil & Robla, 2024; Ni et al., 2025).

## *5. Conclusion*

The convergence of ionic liquids and catalytic hydrogenation technologies is redefining the future of carbon management. By enabling one-pot capture and conversion of $CO_2$ to methanol, IL–catalyst systems exemplify process intensification, offering reduced energy penalties, minimized material losses, and the possibility of modular, distributed methanol production. This integration not only enhances the efficiency of CCUS but also positions methanol at the heart of the methanol economy as both a chemical platform and an energy vector.

Yet, achieving sustainable deployment requires a concerted research roadmap. First, rational design of ILs must go beyond capture efficiency to incorporate reactivity and intermediate stabilization, enabling multifunctional solvents that act as both sorbents and catalytic promoters. Second, catalyst development must address sintering and deactivation pathways in liquid environments while ensuring compatibility with IL matrices, leveraging defect engineering, promoter effects, and advanced supports. Third, reactor engineering must focus on scale-up feasibility and the integration of these systems into modular CCUS units capable of operating under realistic flue gas conditions.

Pursuing these directions will accelerate the transition from laboratory demonstrations to industrially viable platforms, advancing circular carbon management and bridging the gap between climate mitigation targets and chemical manufacturing sustainability.

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