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Catalytic CO_2 Hydrogenation Reactions to Methanol: Catalysis, Intensification and Modelling

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Introduction Efficient CO_2 utilization demands smarter routes to methanol, and conventional hydrogenation is held back by equilibrium limits. In situ removal of methanol and water with ionic liquids (ILs) presents an opportunity to break through these constraints and unlock higher conversions for more robust operation. This work explores the potential of IL-assisted synthesis through targeted IL screening and microkinetic modeling.

Methods Candidate ILs were examined through thermal exposure and sorption tests to evaluate stability, decomposition tendencies, and liquid-phase behavior at elevated temperatures. This was complemented by COSMO-RS predictions of methanol and water solvation to identify ILs with favorable affinity for selective product removal. A multisite microkinetic model [1,2] for CO_2 hydrogenation over Cu-based catalysts was applied to simulate intrinsic reaction rates and assess how IL-driven product extraction influences overall conversion and reactor performance.

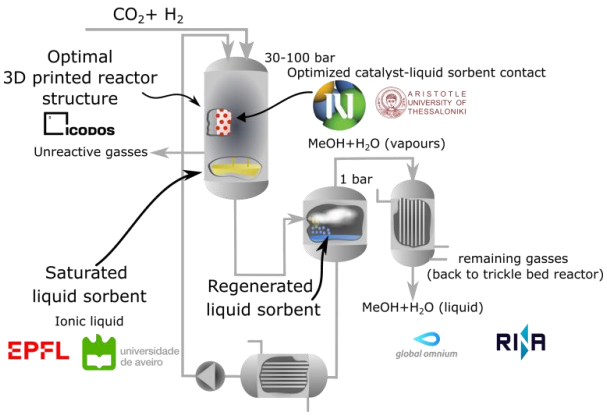

Figure: Process scheme of IL-enhanced methanol synthesis process.

Results and Discussion The combined screening approach identified ILs with relevant thermal stability and sufficient methanol and water sorption capacity, though long-term stability under reaction conditions is still under investigation. These observations have direct implications for reactor design, emphasizing the need to optimally separate IL and catalyst to avoid deactivation while enabling vapor-phase product withdrawal. Microkinetic simulations show that effective in situ removal can substantially improve conversion, but performance depends on IL stability, regeneration capability, and thermal management. Overall, the results support the potential of IL-assisted methanol synthesis while highlighting key constraints that must be addressed in further process development.

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References

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