ADSORBENT DESIGN FOR PROCESS INTENSIFICATION IN CO_2 VALORISATION TO METHANOL

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Abstract. The increasing concentration of atmospheric CO_2 and its impact on climate change have intensified the search for sustainable carbon utilization technologies. Among the available carbon capture and utilization routes, the catalytic hydrogenation of CO_2 to methanol has emerged as a particularly attractive pathway, enabling the production of a versatile chemical feedstock, energy carrier, and platform molecule for a future circular carbon economy (Bukhtiyarova et al. 2017). However, despite significant advances in catalyst development, the direct hydrogenation of CO_2 remains thermodynamically limited, typically achieving only 10–25% methanol conversion per pass under industrially relevant conditions (Reichert et al. 2019). One promising strategy to overcome these limitations is process intensification through in situ product removal. By selectively removing methanol and water from the reaction medium, the reaction equilibrium can be shifted towards higher conversions, reducing recycle requirements and improving overall process efficiency. Within the framework of the Horizon Europe ILIMITED project, ionic liquids (ILs) are being explored as selective absorbents capable of operating directly under methanol synthesis conditions. The design of suitable ILs presents a complex multi-objective challenge. Candidate solvents must exhibit high affinity for methanol and water, low CO_2 absorption to preserve selectivity, low viscosity to ensure efficient mass transfer, and, critically, high thermal and chemical stability at

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temperatures around 513 K. To address this challenge, a computational workflow combining COSMO-RS molecular thermodynamics, large-scale virtual screening, and machine-learning tools was developed to evaluate millions of ionic liquid structures and identify promising candidates. Approximately 19 million ILs were screened, enabling the identification of a small set of promising candidates exhibiting high methanol/water affinity, low CO_2 uptake, and suitable thermal stability for operation under methanol synthesis conditions. These candidates have been selected for experimental validation, including thermal and chemical stability assessments under relevant reaction conditions, to verify their applicability in equilibrium-shifting methanol synthesis processes.

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