

ILIMITED: Understanding Liquid Sorbents for Water at High-Temperatures

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Abstract

- High-temperature H_2O and MeOH sorbents were screened for CO_2 conversion applications.
- Liquid sorbents must combine high product affinity with negligible volatility and high thermal and chemical stability.
- Ionic liquids provide tunable cation–anion chemistry but must retain sufficient uptake at elevated temperatures.
- A vapor-TGA method was developed, enabling rapid determination of stability under realistic conditions and measurement of sorption capacity.

Vapor-TGA (thermogravimetry)

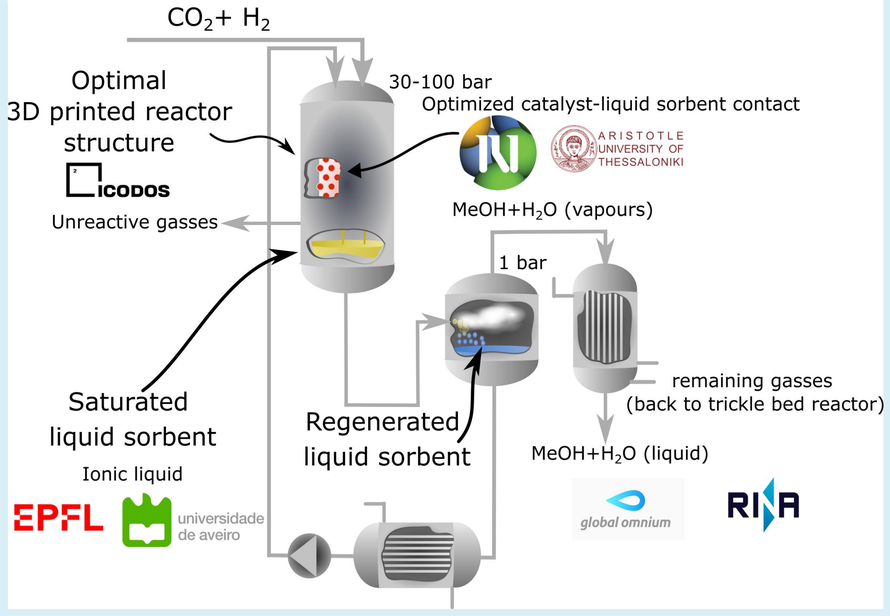


Context

- Use of ionic liquid as sorbents for removal of MeOH and H_2O
- Goal: achieving over 80% CO_2 conversion per reactor pass

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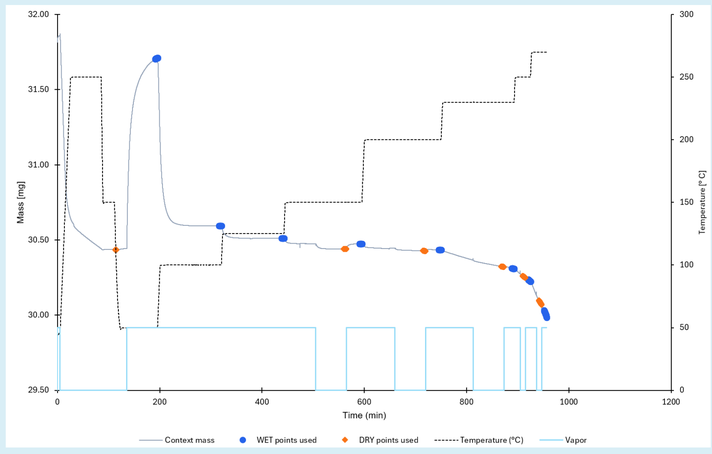
Conceptual process scheme



ILIMITED webpage

Methodology

- Theoretical screening was performed by the University of Aveiro within the ILIMITED project.
- Selected candidates were validated by temperature-programmed Thermogravimetric analysis under vapor exposure using a TA Q50 equipped with an automatic sampler
- Candidates were ranked according to sorption performance and stability under steam conditions relevant to CO_2 conversion.



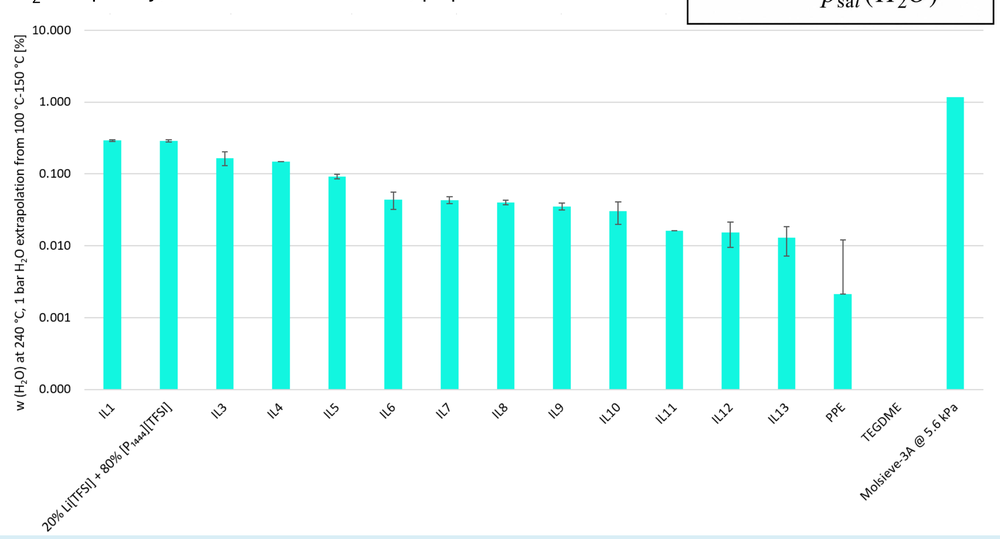
Results and discussion

Sorption capacity measured between 100 °C and 150 °C

- Benchmarks: Molecular sieve 3A, TEGDME (tetraethylene glycole dymethyl ether), olyphenyl ether and UiO-66 composite.
- Results: Li^+ in 20% Li[TFSI] + 80% $[P_{1444}]$[TFSI] provides strongest interaction with H_2O as predicted by COSMO-RS.

$$c = K \frac{p(H_2O)}{p_{sat}(H_2O)}$$

- c… H_2O capacity, K.. interaction factor, p…pressure

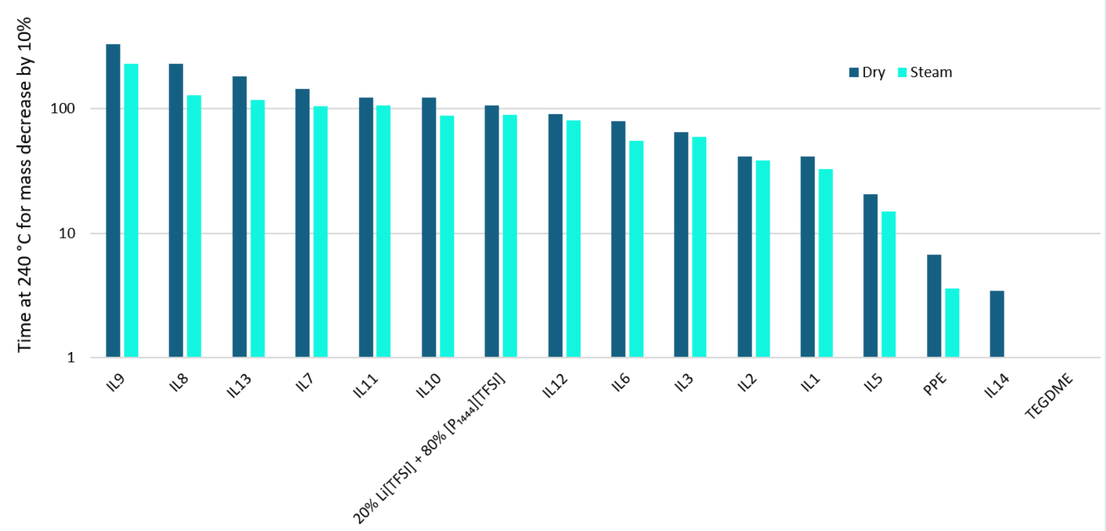


Stability under steam conditions

- Ionic liquids (ILs) are the most thermally stable group of flowing liquids at elevated temperatures of up to 270 °C tested.
- 20% Li[TFSI] + 80% $[P_{1444}]$[TFSI] also shows high stability among other candidates.
- Steam flow increases mass-loss rate by up to **90%.**

- Model equation: first order kinetics of degradation: L…weight change, A preexponential factor, Ea… exponent, t… time, T… temperature

$$t = \frac{-\ln(1-L)}{A} \exp\left(\frac{E_a}{RT}\right)$$



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