QUEEN'S UNIVERSITY BELFAST

QUEEN'S UNIVERSITY IONIC LIQUID LABORATORIES QUILL

CO_2 Capture from Commercial Flue Gas Process Streams;

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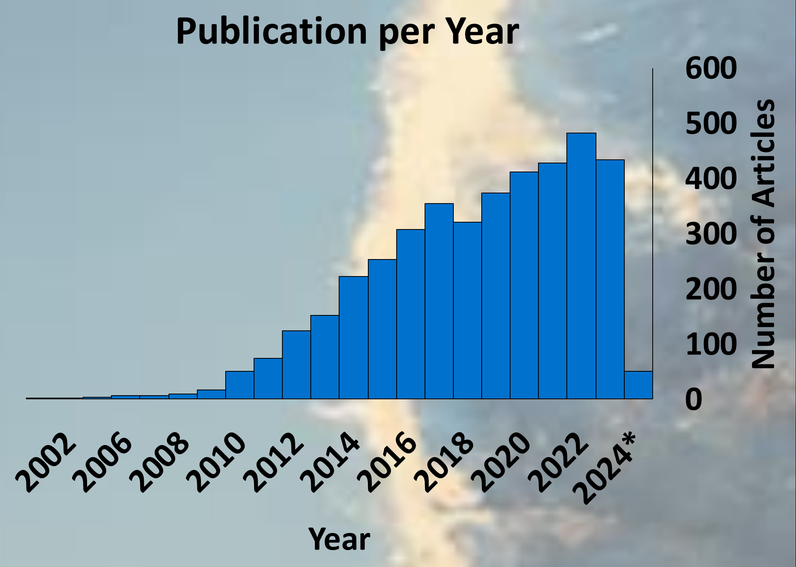
Interactive Database

Ionic liquids (ILs) for the capture of carbon dioxide (CO_2) has become an increasing studied topic. With this database we aim to have an up-to-date compilation of the available chemisorption data for CO_2 capture. With an extensive delve into the available literature, ILs have been incorporated into many technologies including application in membrane separation, amine scrubber blends, porous liquids, deep eutectic solvent (DES) and their capabilities as CO_2 physisorbent but this database will primarily focus on their CO_2 chemisorption capabilities.



Increasing area of research totalling 4,084 papers, 600 papers for further screening est. 200 papers to be added with multiple ILs,

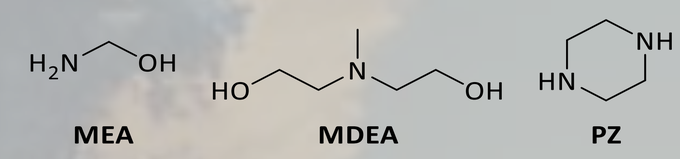
*Web of Science search for 'Ionic Liquids for CO2 Capture' as of March 2024

CO_2 in flue gas

The amount of CO_2 in flue gas varies depending on the initial process. For this project we will be concentrating on flue gas from oil refinery process streams with a typical amount of CO_2 in flue gas around 4%. The main component is N_2 along with water vapour, many impurities (SO_x & NO_x) have already been removed.

Current Technology

The industrial standard currently used for CO_2 capture are amine scrubbers most typically 30 wt% blend of monoethanolamine (MEA) and water. ILs and other amine additives (methyldiethanolamine (MDEA) & piperazine (PZ) have been blended into the system to alleviate some of the drawbacks namely lowering the energy required for release of the captured CO_2. However these amine still susceptible to degrade into corrosive by-product hence the continued effort to find viable alternatives



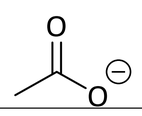
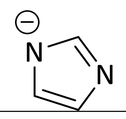
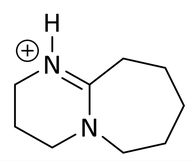
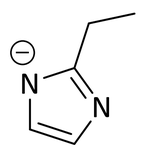
Database Extract

Paper #	Ref.	Cation	Anion	M_w (g/mol)	Water Content (wt%)	Pressure (mbar)	Absorb. Temp. (K)	CO_2 mol/mol absorbent	CO_2 mol/kg absorbent	CO_2 g/kg absorbent	Mole Fraction	Vis. Pre CO_2 (mPa.s)	Vis. Post CO_2 (mPa.s)	Desorb. Temp. (K)
37	a	[DBUH]	[Im]	220.32	N/A	1000	313.8	0.68	3.09	154.00	0.40	18	N/A	N/A
42	b	[DBUH]	[2-EtIm]	248.38	N/A	1000	313.0	0.50	2.01	88.57	0.33	N/A	N/A	N/A

This interactive database aims to capture and correlate important parameters that influence the capacity of CO2 capture and industrial application; operating temperatures, pressure, viscosity. The presence of water is an important consideration to industrial application. Title and DOI also included in the database but exempt from the extract. Using excel functions able to determine different parameters with data reported. When only graphs are presented in papers authors are contacted via email for the numerical data.

References: a) *Sep. Pur. Tech. 263 (2021) 118417* b) *ACS Sustainable Chem. Eng. 2017, 5, 8192−8198*

Structural Database Extract

Standard Abbreviation	Paper Abbreviation	Name	Structure	Keywords	Cation/ Anion	M_w (g/mol)	Mentioned in Entries	Entry #	
[OAc]	[acetate], [OAc]	Acetate		Oxygen	A	59.04	26, 58	26	58
[Im]	[Im]	Imidazolate		5 membered ring, nitrogen	A	67.07	17, 37, 42	17	37
[DBUH]	[DBUH]	8-diazabicyclo[5.4.0]undec-7-ene		Bicyclic, 5 & 7 membered ring, nitrogen	C	153.25	37, 58, 42	37	58
[2-EtIm]	[2-EtIm]	2-ethyl-imidazolate		Substituted imidazole ring, nitrogen	A	95.13	37	37	

We have designed and compiled an interactive structural database to enable us to spot trends in reactivity among chemisorbent ILs with the further goal of designing novel ILs for chemisorbent CO_2 capture of flue gas. This database has the potential to offer AI valuable insights into advancements in carbon capture

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