Ministero dell'Università e della Ricerca

FIS

POLITECNICO MILANO 1863 | DEPARTMENT OF ENERGY

Selection of Ionic Liquids for CO_2 Capture

A practical screening funnel for ionic liquids in CO_2 bubble-column absorption

24.08.2026 I Alberto Arici

AURIGA project – The goals

AURIGA - Unveiling the RIddles of GAs-liquid fluid dynamics

Towards novel carbon dioxide absorption systems

General Goals

Formulate a **novel theory** to unveil some of the riddles (e.g., multi-scale connections) of **gas-liquid fluid dynamics** and apply the acquired perspective to develop a novel **ionic-liquid reactor** to absorb **carbon dioxide** from sour gas streams.

Specific Goals

1. Develop a **physical-based approach** to describe a-priori the flow patterns in **bubble columns**, including the relationships between local and global flow properties;
2. Set-up **experimental facilities** (small-scale and large-scale) to study the influence of **ionic liquids** on the local and the global fluid dynamics and to study the mass transfer in ***CO_2-IL* systems**;
3. Scaling-up towards the industrial scale.

AURIGA project – The Team

Principal Investigator
Prof. Giorgio Besagni, PhD

Post Docs

Nicolò Varallo

Stefano Puricelli

Khaled Gad

PhDs

Andrea Ferrario

Alberto Arici

Vitor Regert

Djamel Aissaoui

Francesco Pierini

AURIGA project – The Team @ CHISA2026

Post Docs

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Vitor Regert

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Francesco Pierini

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Andrea Ferrario

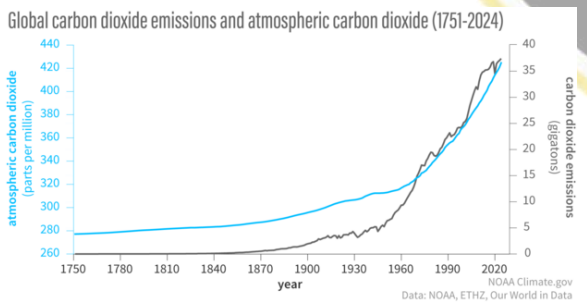
Motivation & Aim

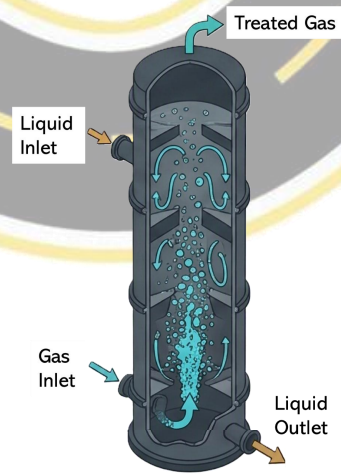
CO_2 emissions are a major climate challenge, requiring scalable capture solutions

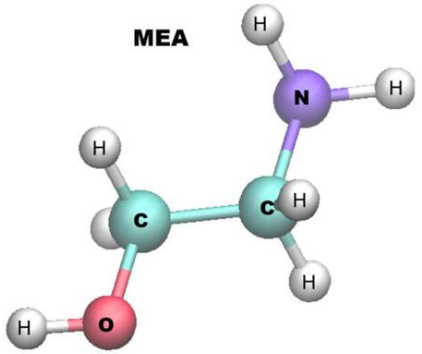
Chemical absorption in **gas-liquid processes** is the most mature technology for CO_2 capture

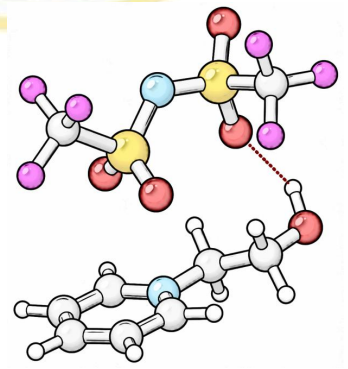
Conventional amine systems are effective but suffer from several **drawbacks**

Ionic liquids have emerged as promising alternative









[1] Nunes (2023), Enviroments
[2] Rochelle (2009), Science
[3] Hospital-benito et al. (2020), Chemical Engineering Journal

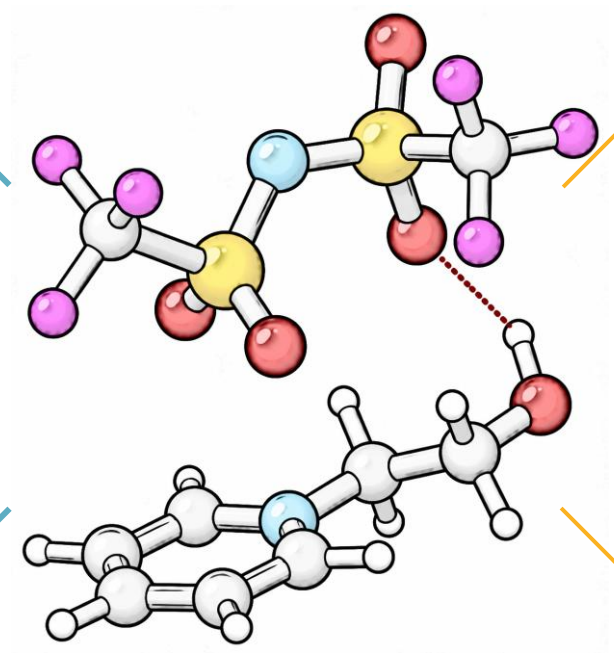
The Ionic Liquid Promise

Infinite Tunability

Over **10^{14} possible cation/anion combinations** allow precision engineering of viscosity, capacity and thermal properties

High stability

High thermal and chemical endurance allows for alternative **high-efficiency regeneration** strategies like flash desorption



Zero vapor pressure

ILs do not evaporate eliminating **solvent losses** and atmospheric emission entirely

Selective affinity

Exceptional physical and chemical **affinity for CO_2** over a lot of other gases

[3] Hospital-benito et al. (2020), Chemical Engineering Journal
[4] Chiappe et al. (2005), Journal or Physical Organic Chemistry
[5] Wassercheid et al (2002)

The Ionic Liquid Promise

Infinite Tunability

Over **10^{14} possible cation/anion combinations** allow precision engineering of viscosity, capacity and thermal properties

The real research question

Which ionic liquids are worth testing in the actual reactor, under actual mass-transfer limitations?

From infinite possibilities to testable candidates

Huge IL design space
Cation–anion combinations and functionalization create an almost "infinite" design space.

AI-assisted literature mapping
What has already been experimentally characterized?

Physics-based screening
Which properties actually matter for CO_2 capture?

Thermodynamic Modelling
Can we predict/complete missing equilibrium information?

Reactor-oriented assessment
Will a promising solvent still perform in a bubble column?

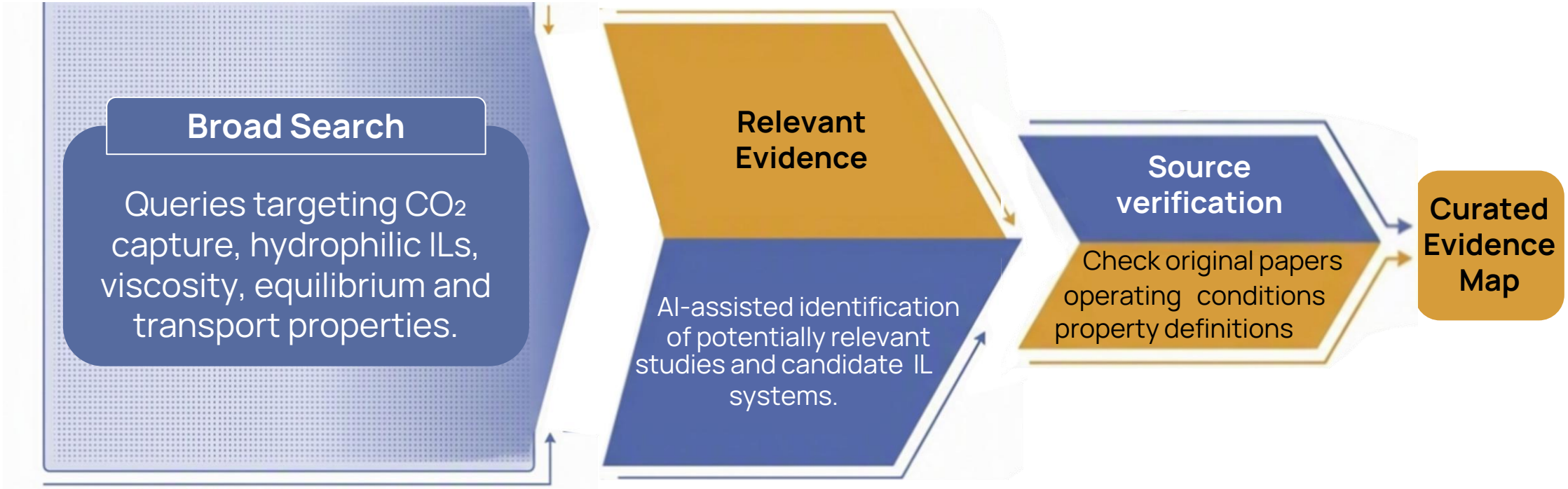
Selected Candidates

A small set of feasible systems for detailed experimental and modelling studies

[6] Borhani et al. (2019), *Renewable and Sustainable Energy Reviews*
[7] Foorginezhad et al. (2022), *Frontiers in chemistry*

Step 1 – AI-assisted literature mapping

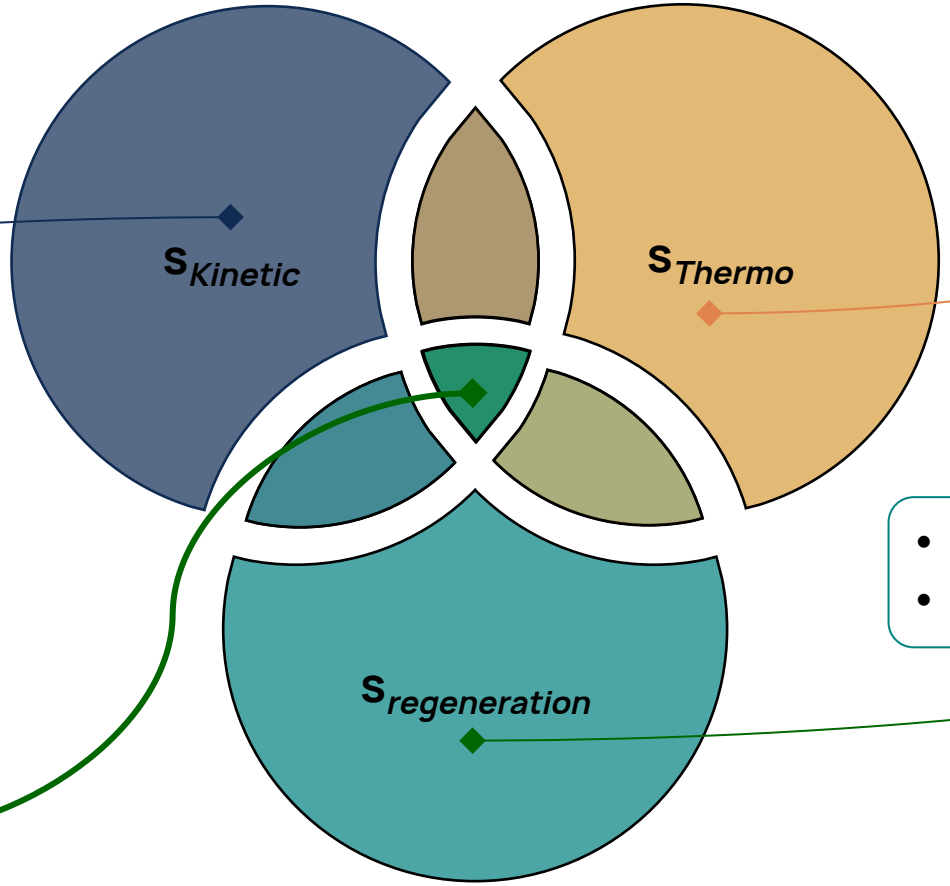
Available evidence is broad but fragmented, making a structured mapping step necessary before screening.



Conclusion: AI accelerates evidence discovery, while final data selection remains source-verified.

[8] Torralba-Calleja et al. (2013), *journal of Chemistry*

Physics based screening indicators



- CO2 affinity $1/H$
- Working capacity / loading

- Viscosity: μ
- CO2 diffusivity: D_{CO_2}
- Cosolvent compatibility

- Absorption enthalpy: $|\Delta H_{abs}|$
- Stability

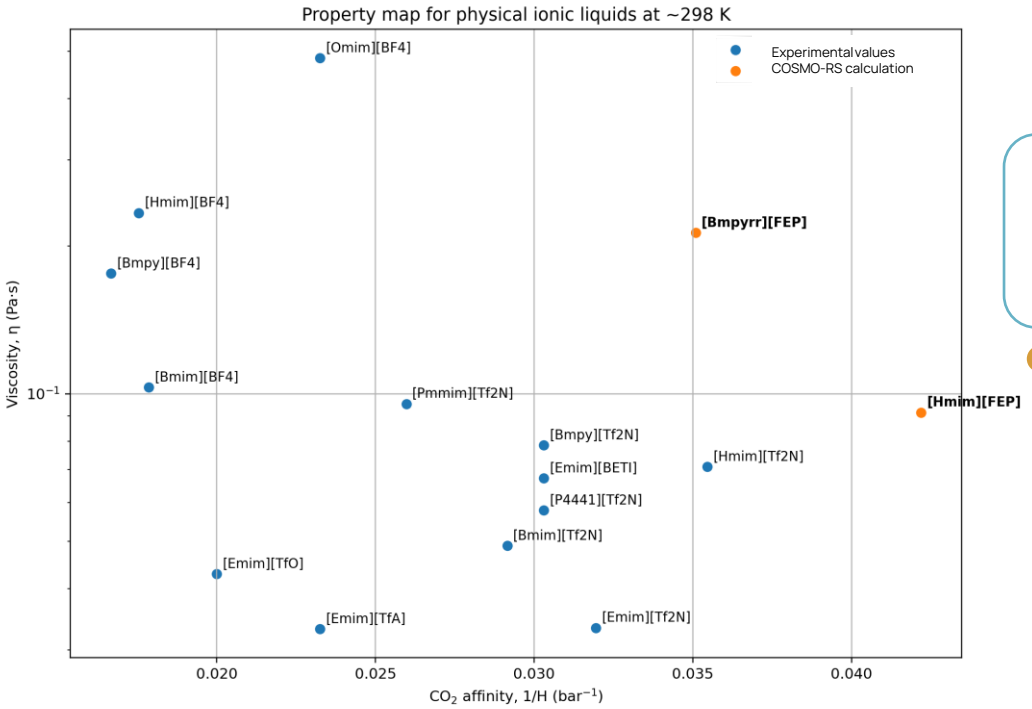
BEST COMPROMISE!

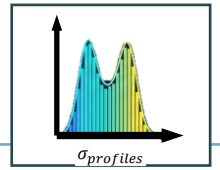
Overall screening score: $w_T S_{Thermo} + w_K S_{Kinetic} + w_R S_{Regeneration}$

[6] Borhani et al. (2019), *Renewable and Sustainable Energy Reviews*
[9] Gurkan et al. (2010), *The journal of physical chemistry Letters*
[10] Zeng et al. (2017), *Chemical reviews*

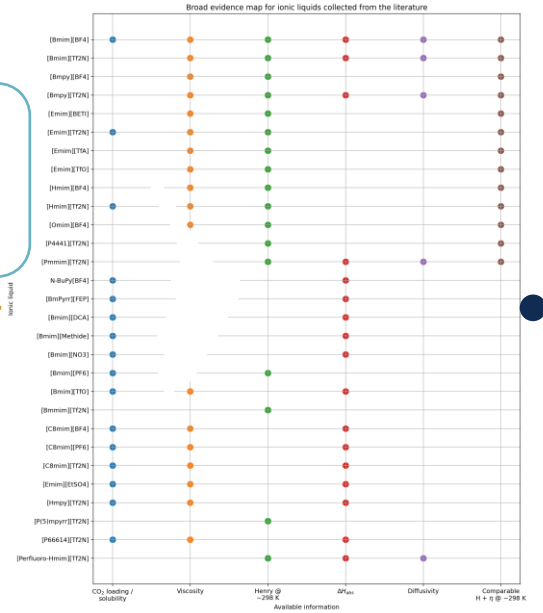
From fragmented evidence to comparable properties

Available evidence is broad but fragmented, making a structured mapping step necessary before screening.





Thermodynamic models can complement missing data and provide consistent property estimates for screening.



Curated Evidence Map

Conclusion: AI accelerates evidence discovery, while final data selection remains source-verified.

[11] Hou et al. (2007), *Industrial & Engineering Chemistry Research*
[12] Moganty et al. (2010), *Industrial & Engineering Chemistry Research*
[13]Zhang et al. (2008), *AIChE Journal*

The kinetic penalty

High affinity on paper

Poor transport in practice

The Trap

Relying on Henry's constant or equilibrium solubility (x_{CO_2}) suggest Functionalized ILs are universally superior.

The Reality

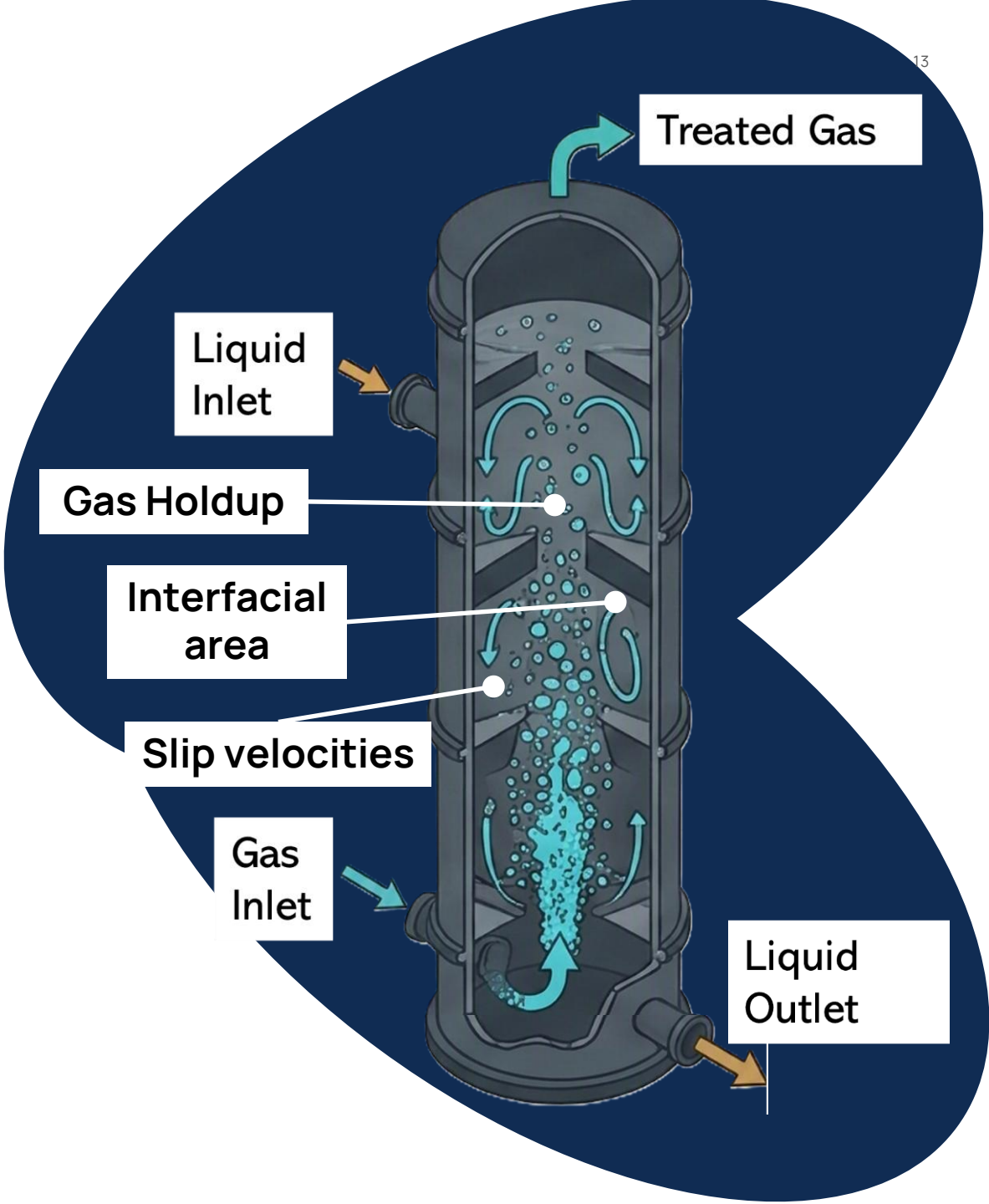
CO_2 absorption is kinetically controlled. High viscosity reduces the liquid-side mass-transfer coefficient (k_L)

[9] Gurkan et al. (2010), *Journal of Physical Chemistry Letters*
[13] Zhang et al. (2014), *AIChE Journal*
[14]Santiago et al. (2018), *Chemical Engineering Journal*

Reactor-oriented assessment: 1D- two fluid model

The Fluid dynamic Imperative in bubble columns

Surviving candidates face the critical bottleneck: **the reactor**. We evaluate different solvents under identical geometry and operating conditions using a transient, one dimensional **Euler-Euler two fluid model.** Static metrics are useless without resolving the fluid dynamcs.



[13] Zhang et al. (2014), *AIChE Journal*
[15] Besagni et al. (2018), *ChemEngineering*

Final selected system

Performance indicators +

Toxicity / HSE

Cost / procurement

[BMIM][BF_4]

reference system for physical absorption

- Benchmark physical ionic liquid
- Literature-rich system for comparison
- Compatible with CFD / hydrodynamic studies
- Feasible procurement and lab-scale handling

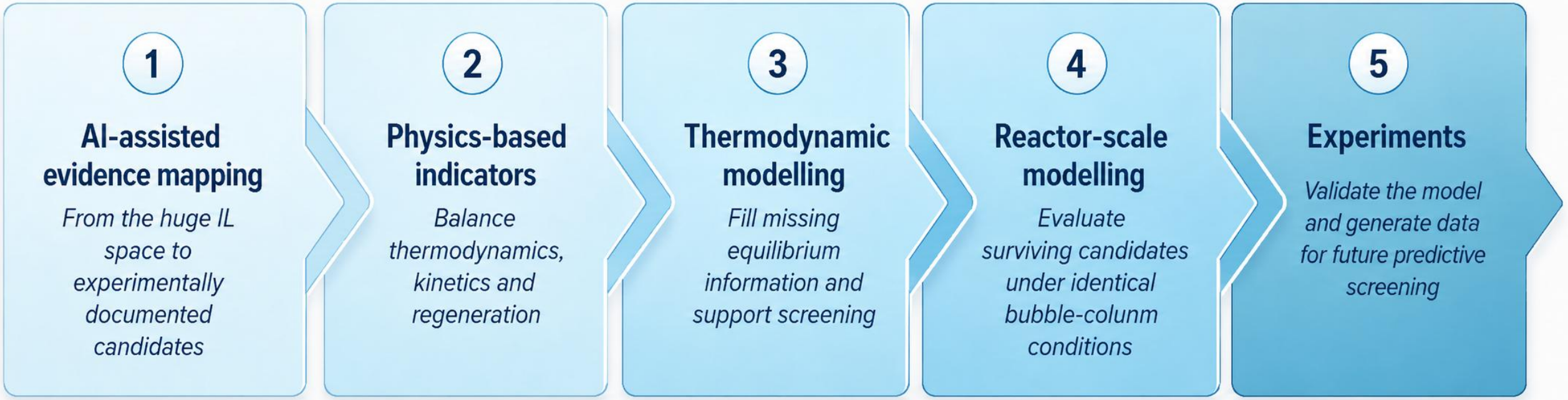
[EMIM][OAc]

high-affinity hydrophilic system

- Hydrophilic system for aqueous mixtures
- High CO_2 affinity / chemically enhanced uptake
- Relevant to co-solvent viscosity-reduction strategies
- Complementary case to [BMIM][BF_4]

[10] Zeng et al. (2017), *Chemical reviews*
[16] Shiflett et al. (2010), *Energy & Fuels*

Summary and conclusion



Thank you for the attention

Acknowledgment

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Contatti

alberto.arici@polimi.it

LinkedIn