Feasibility of the microwave regeneration of impregnated adsorbents for carbon capture

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1. WLA Process for Carbon Capture

The 'Wetting Layer Absorption' (WLA) process[1,2] is a novel concept which attempts to combine the positive aspects of adsorption and absorption for application in post-combustion carbon capture. A porous material is used to support liquid-like regions of absorbed solvent which in turn absorb carbon dioxide.

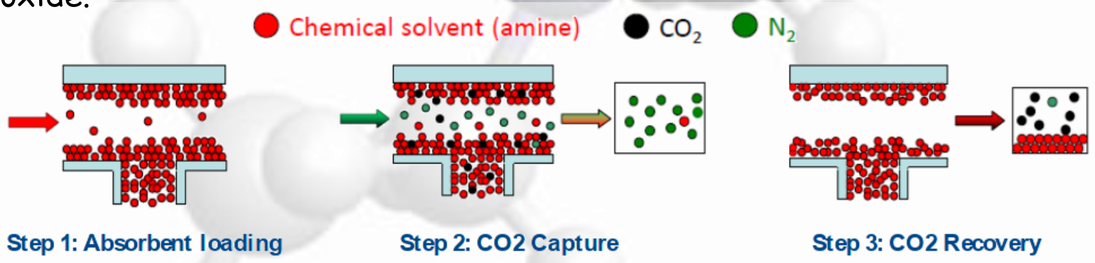
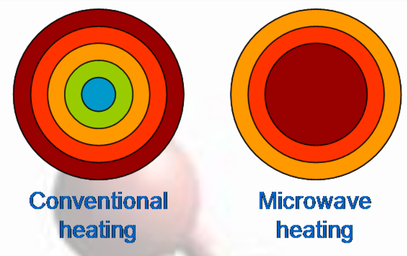


Figure 1: WLA process

Advantages of the WLA process:
- Increases interfacial area vs standard absorption process.
- Solvent partial pressure is optimized.
- Potential use and optimization of physical or chemical solvents.
- Lower regeneration penalty than amine scrubbing tower (no water).

2. Microwave heating

Advantages of microwave heating:
- Volumetric heating → much faster.
- Targeted heating → much more efficient.
- Operates at lower temperatures.
- Reduces leaching and sorbent degradation.



Heat absorbed from microwaves

Maxwell's Equations

$$\vec{\nabla}\cdot\vec{D}(r,t)=4\pi\rho_e(r,t)$$
$$\vec{\nabla}\cdot\vec{B}(r,t)=0$$
$$\vec{\nabla}\times\vec{E}(r,t)=-\frac{1}{c}\frac{\partial\vec{B}(r,t)}{\partial t}$$
$$\vec{\nabla}\times\vec{H}(r,t)=\frac{4\pi}{c}\vec{J}_e(r,t)+\frac{1}{c}\frac{\partial\vec{D}(r,t)}{\partial t}$$

$$Q_{abs}=\frac{\omega}{4\pi}\varepsilon''(\omega)|\mathbf{E}|^2V$$

ω: angular frequency
ε''(ω): imaginary part of the dielectric constant
|E|: strength of electric field
V: volume of the system

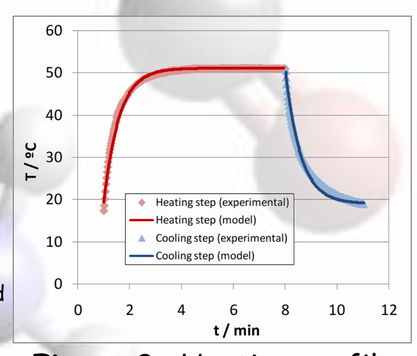


Figure 2: Heating profile

3. Determination of the frequency-dependent dielectric constant

Dielectric constant

$$\varepsilon(\omega)=\varepsilon'(\omega)+i\varepsilon''(\omega)$$

ε'(ω): Ability to store potential energy by being polarized by an electric field
ε''(ω): Dielectric loss, electromagnetic energy is transformed into heat due to collisions

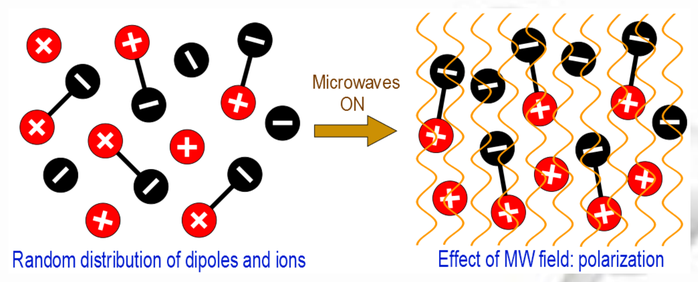


Figure 3: Dielectric heating

The dielectric constant of a medium is related to the fluctuations in the dipole moment of the system:

$$\frac{\varepsilon(\omega)-\varepsilon_\infty}{\varepsilon_0-\varepsilon_\infty}=1+i\omega\hat{\phi}(\omega)$$

ϕ (ω): Fourier transform of the dipole moment autocorrelation function

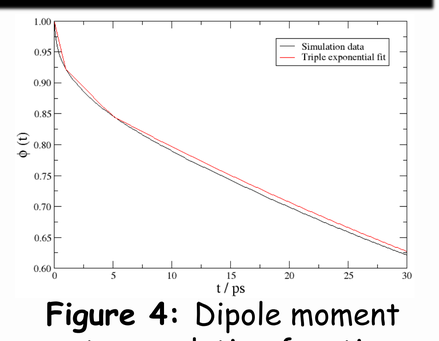


Figure 4: Dipole moment autocorrelation function

4. Molecular Dynamics simulations

In Molecular Dynamics (MD) simulations, atoms and molecules are allowed to interact, and their trajectories are determined by integrating Newton's equations of motion. The forces acting in the system are defined through parameterized sets of equations called force fields. In this work, MD simulations are performed using the software GROMACS[3] to analyze the interactions between molecules of different solvents and determine their dielectric properties.

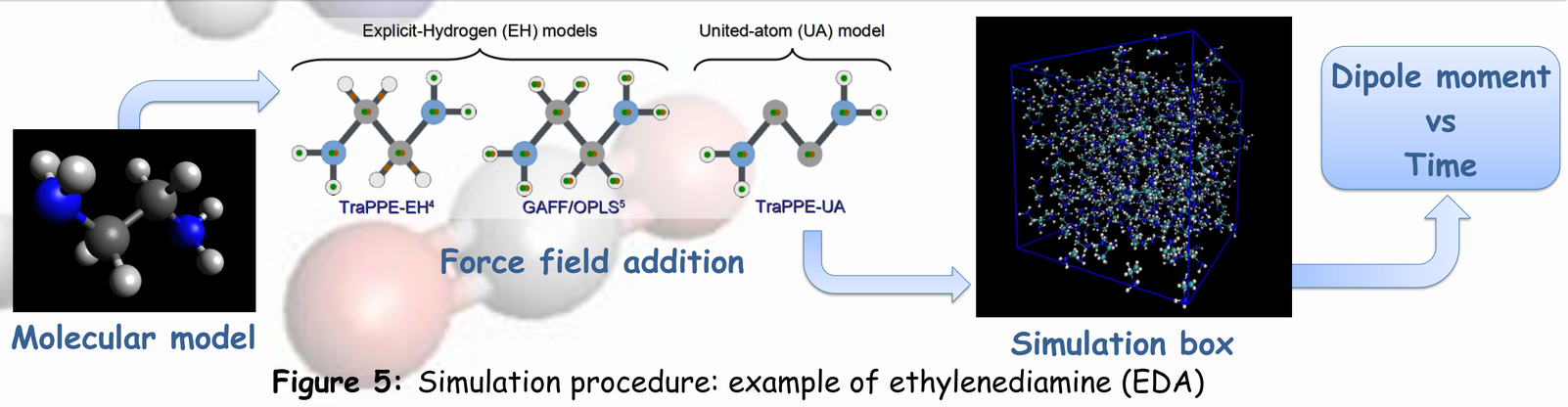


Figure 5: Simulation procedure: example of ethylenediamine (EDA)

5. Results – Dielectric spectra

Little data have been found in the literature for the frequency dependence of the dielectric constant of solvents of interest in carbon capture. Because these are essential to ascertain the feasibility of the microwave regeneration process , our objective is to obtain the required properties by means of MD simulations.

Ethanol

Ethylenediamine (EDA)

Spectra Comparison

- The more polar the solvent, the highest the peak in ε'' (ω).
- The larger the solvent, at the lower frequency absorption occurs.

6. Future work

- Validate method with more solvents
- Analyze the effect of pore confinement on dielectric constant.

7. References

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8. Acknowledgments

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