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Experimental determination and modeling of diffusion coefficients as a function of the composition of binary mixtures of CO_2 and ethanol

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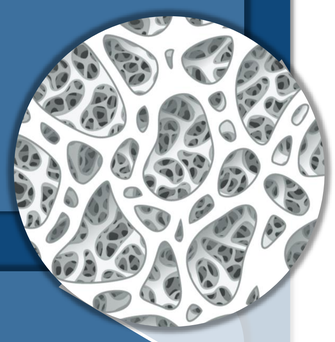
Experimental determination

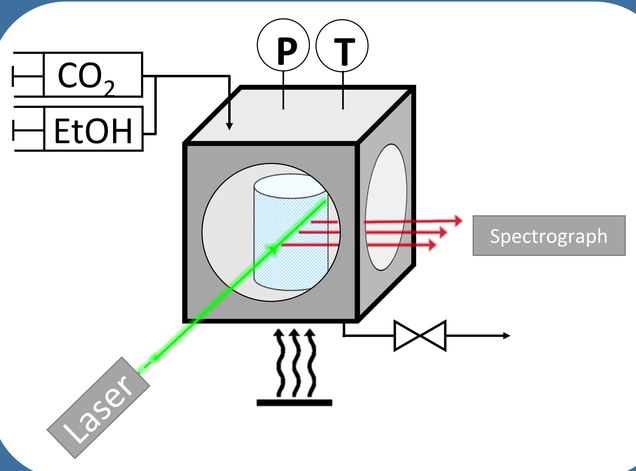
Mass transfer in open porous structure

- ✓ Pore size = 35-50 nm
- ✓ High capillary forces
- ✓ Prevention of free convection
- ✓ Only diffusional mass transfer



High-pressure view cell

$P = 80 - 120$ bar & $T = 308 - 333$ K

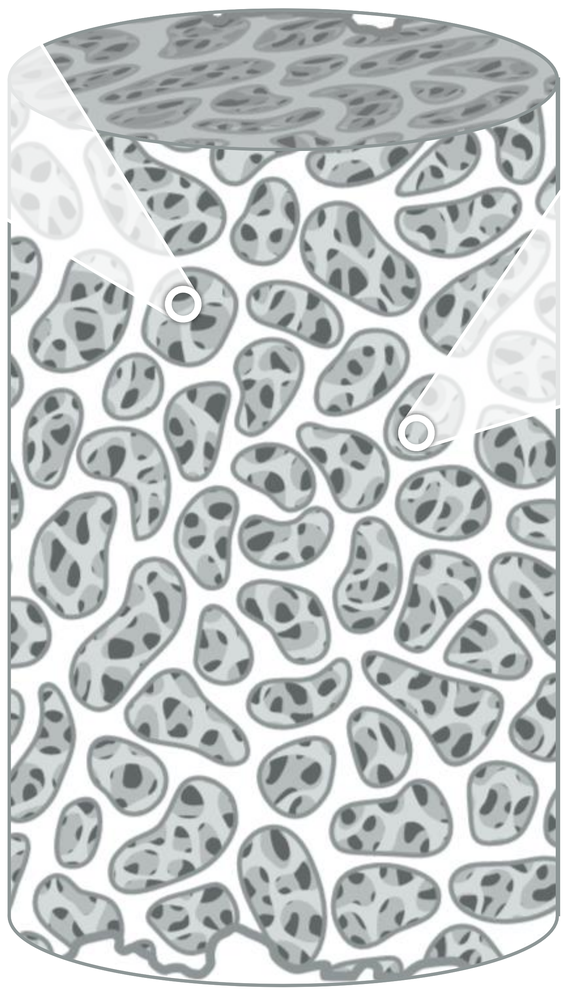


Mass transfer model

- ✓ 1D-radial Diffusion & volume change upon mixing
- ✓ Stepwise Region-of-Interest scanning and fitting

Motivation

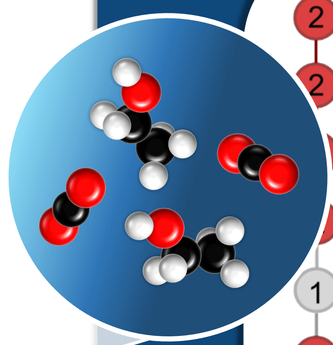
- ✓ Lack of composition dependent diffusion coefficients
- ✓ Measurement is complex in mixture of solvent & CO_2 due to non-ideality
- ✓ Accurate data for design and optimization of extraction processes
- ✓ Simple correlations fail for non-ideal mixtures

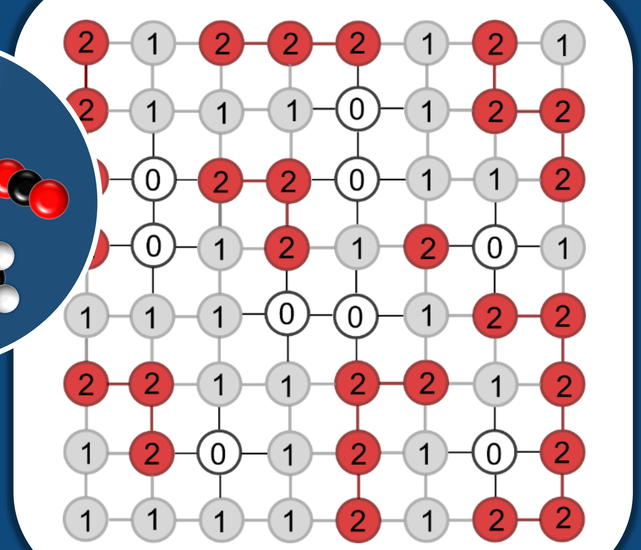


Thermodynamic modeling

Mixture Density Correlation

- ✓ Non-Random Hydrogen Bonding (NRHB) Model
  - ✓ Compressible Lattice-Fluid
  - ✓ non-random distribution of species
  - ✓ hydrogen bonding





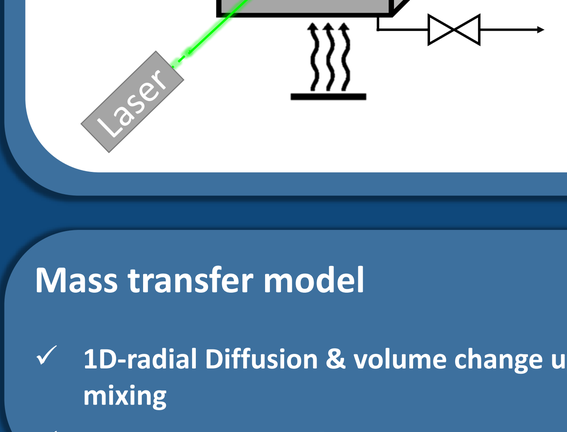
Thermodynamic correction factor

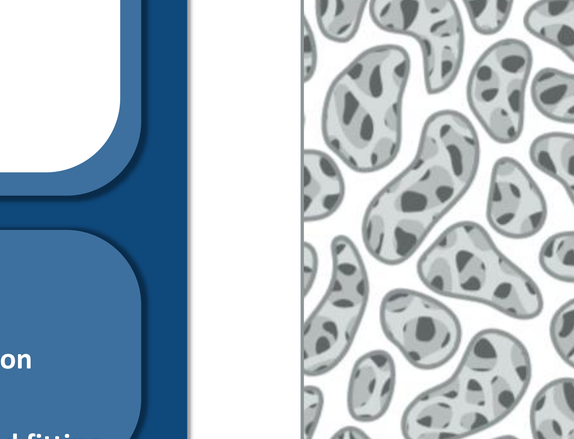
$$\Gamma = \left(1 + x_1 \cdot \frac{\partial \ln \gamma_1(p, T, x_1)}{\partial x_1}\right)$$

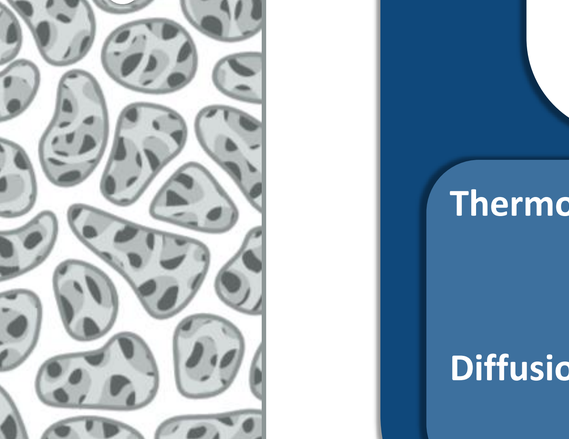
Diffusion coefficient

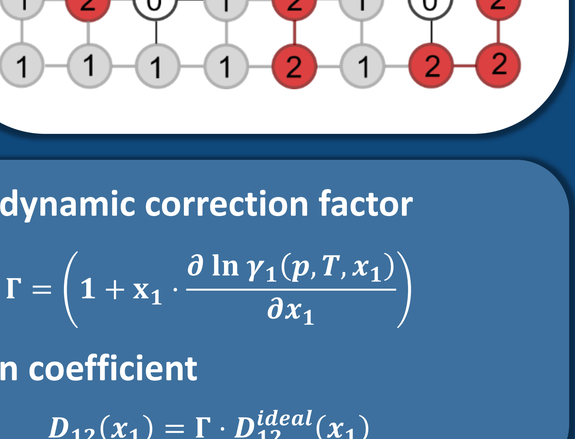
$$D_{12}(x_1) = \Gamma \cdot D_{12}^{ideal}(x_1)$$

Results









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