

# Effect of cavity formation in aqueous solution on gas solubility

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Controlling Emergence

CO<sub>2</sub> solubility is controlled by the cavity formation in the aqueous solutions



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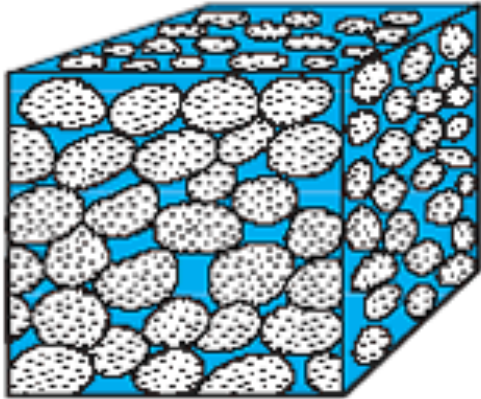


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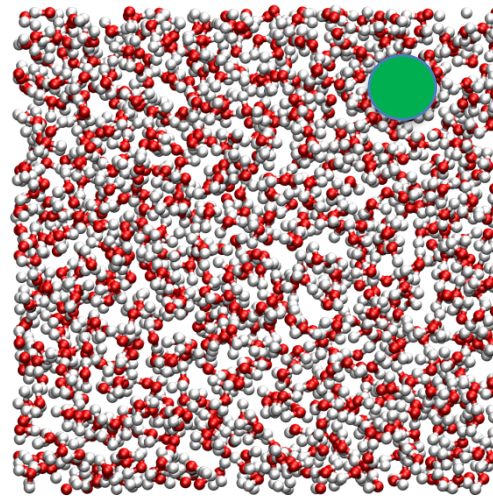


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# Cavity in aqueous solution



Sand - Porosity  
Large scale



Water - Cavity  
Small scale

Probe volume  $R=3.3\text{\AA}$

Density of water: 1g/ml  
→ 5 water molecules in  
the probe volume

Zero water → **cavity**

## Hypothesis:

If there are more cavities (the same size as a gas molecule)  
there will be more gas molecules dissolved in water.

NaCl solution will create fewer cavities than pure water  
because of the strong hydration shell → smaller gas  
solubility



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# Effect of cavity formation on gas solubility

Energy to create the cavities in aqueous solutions

Solubility of CO<sub>2</sub> in aqueous solution at 298K, 1atm

*(Yasunishi and Yoshida, 1979)*

CO<sub>2</sub>, 298K

CO<sub>2</sub>, 308K

CH<sub>4</sub>, 298K



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# Planned Manuscripts

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**Tuan Anh Ho, *Effect of cavity formation in aqueous solution on gas solubility (2018)***



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**Thank you!**

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