Gas transport behavior of isotactic-polypropylene and bio-banking: A molecular dynamics simulation approach

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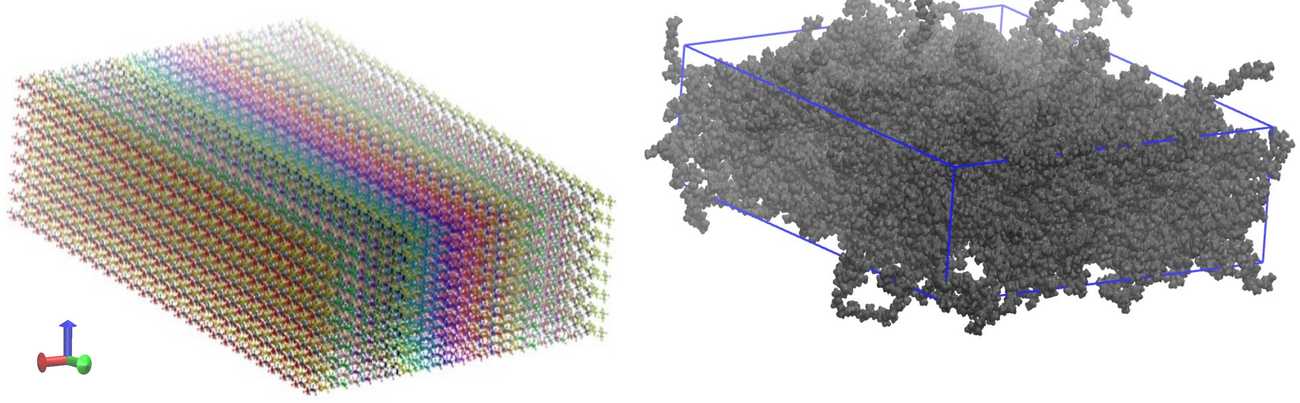
Introduction:

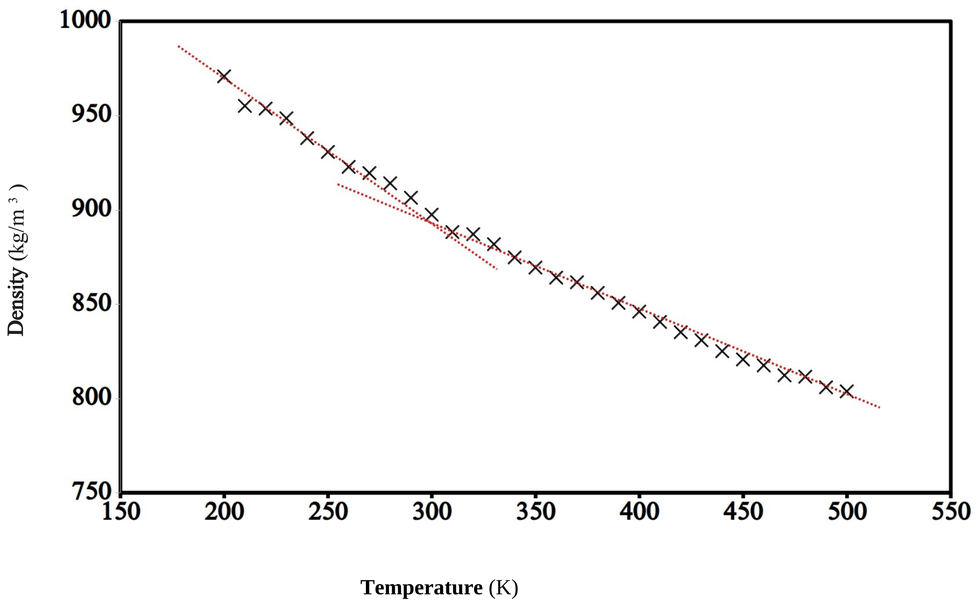
Isotactic polypropylene (i-PP) is widely utilized in medical and laboratory applications, due to its high rigidity, good chemical resistance, and suitability for sterilization.(1) The gas penetration behavior of i-PP plays a crucial role in preserving the stability and integrity of biological samples, making it a valuable material for biobanking.(2)

A “biobank” is defined as an organized process for the long-term storage of biological samples and associated data to support diverse research purposes.(3)

1) Design iPP

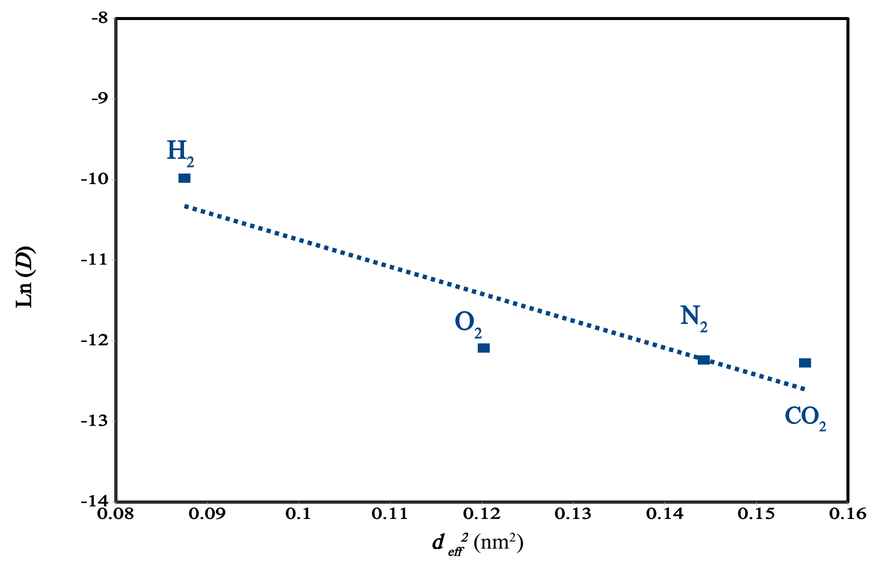


2) FF parameters validation for iPP



3) Gas Diffusion calculation (*D*)

- 5 molecules of gas
- 10ns , **NVT**
- 300 K , 1 atm
- **CHARMM36**



4) Gas Solubility calculation (*S*)

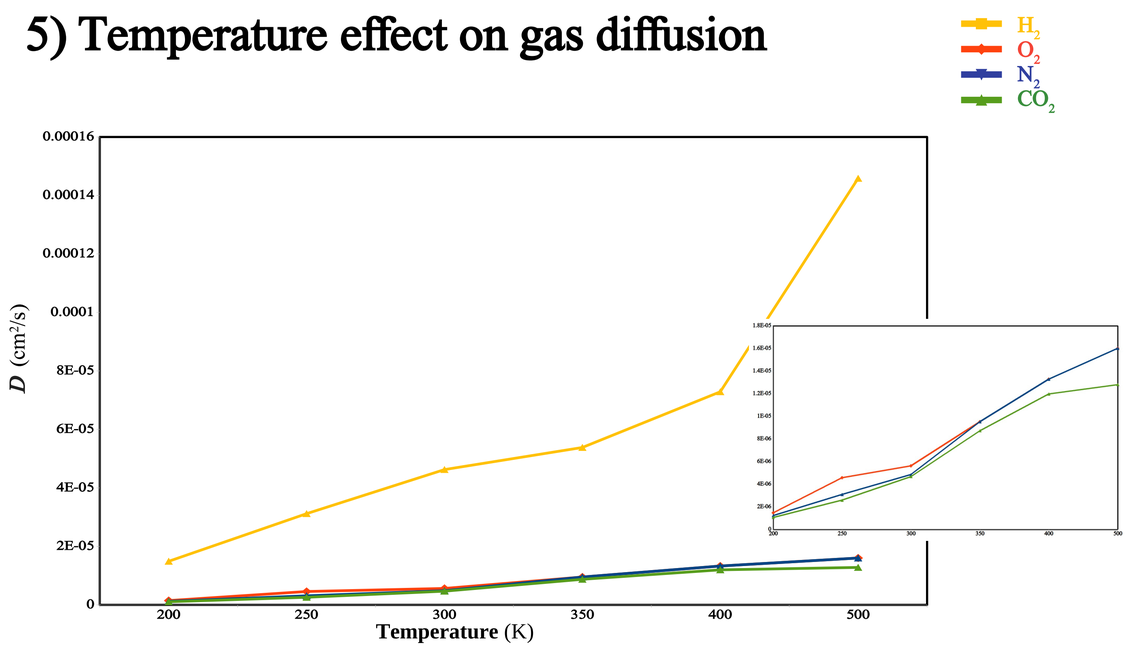
A) ΔG_{abs} CO_2 in FEP (Bennett Acceptance Ratio-BAR)

B) ΔG_{abs} CO_2 in TI

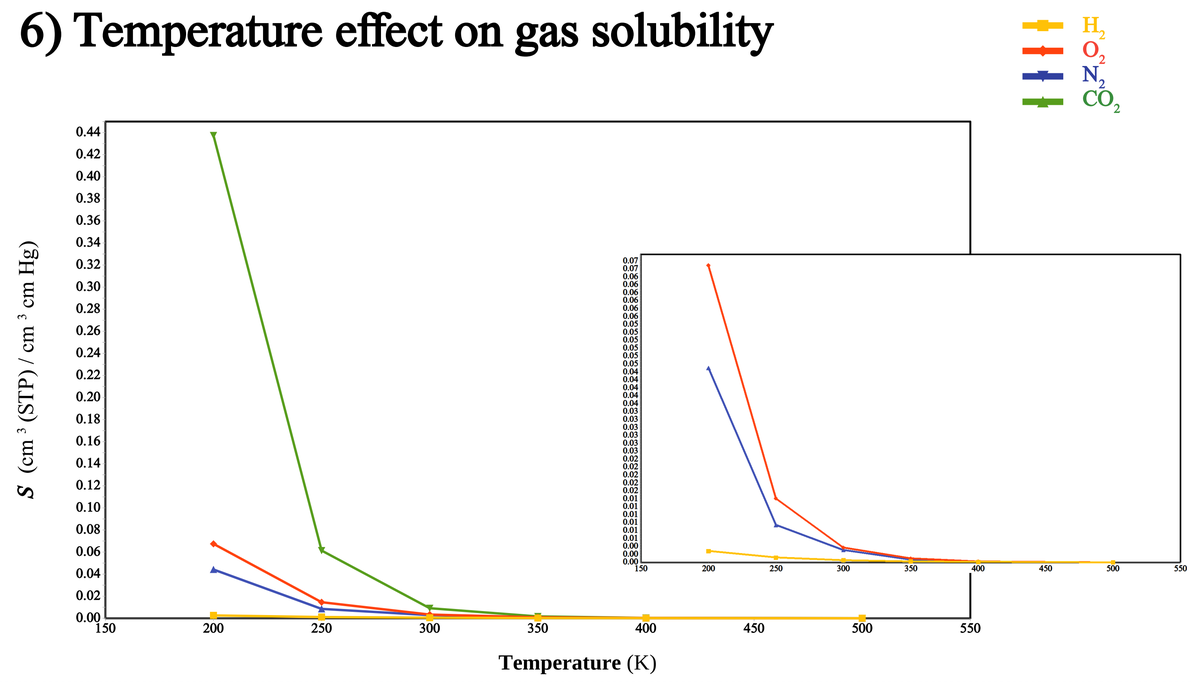
C) μ_{ex} CO_2 in TPI

Method	ΔG_{abs} or μ_{ex} (kJ/mol)	*S* at 300K (cm 3 (STP) / cm 3 cm Hg)
TI	≈ -1.14	18.18×10^{-3}
FEP	≈ - 0.97	17.67×10^{-3}
TPI	≈ 0.68	9.10×10^{-3}
Experimental(4)		3.07×10^{-3}
Other MD(5)		0.41×10^{-3}

5) Temperature effect on gas diffusion



6) Temperature effect on gas solubility



References:

(1) K. Gai, X. Ren, J.Chen, X. Zhou, Q.Wan, Qi Wang, Y. Li, Construction of Helically Oriented Syndiotactic Polypropylene/Isotactic Polypropylene Composites for Medical Interventional Tubes via Rotation Extrusion, Industrial & Engineering Chemistry Research , Volume 62, Number 2 , 2022

(2) O.Malykh, A. Golub, V. Teplyakov, Polymeric Membrane Materials: New Aspects of Empirical Approaches to Prediction of Gas Permeability Parameters in Relation to Permanent Gases, Linear Lower Hydrocarbons and Some Toxic Gases, Colloid Interface Science, Volume 164, Number 1-2, 2010.

(3) R.Hewitt, P.Watson, Biopreservation and Biobanking, Volume 11, Number 5, 2013

(4) V.Siracusa, I.Blanco, S.Remani, U.Tylewicz, Gas Permeability and Thermal Behavior of Polypropylene Films Used for Packaging Minimally Processed Fresh-Cut Potatoes: A Case Study, Journal of Food Science, Volum 77, Number 10, 2012

(5) S.Pricle, M.Fermeglia, Atomistic molecular dynamics simulations of gas diffusion and solubility in rubbery amorphous hydrocarbon polymers, Chemical Engineering Communications , volume 190, Number 10, 2003