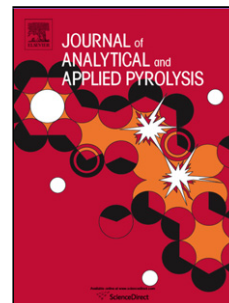


Accepted Manuscript

Title: Diffusion of CO₂ and Fractional Free Volume in Crystalline and Amorphous Cellulose

Authors: Abdul Salam Mohammad, Joseph J. Biernacki, Scott. Northrup, Michael Adenson



PII: S0165-2370(16)30534-4
DOI: <https://doi.org/10.1016/j.jaap.2018.05.005>
Reference: JAAP 4324

To appear in: *J. Anal. Appl. Pyrolysis*

Received date: 9-9-2016
Revised date: 2-5-2018
Accepted date: 8-5-2018

Please cite this article as: Abdul Salam Mohammad, Joseph J. Biernacki, Scott. Northrup, Michael Adenson, Diffusion of CO₂ and Fractional Free Volume in Crystalline and Amorphous Cellulose, Journal of Analytical and Applied Pyrolysis <https://doi.org/10.1016/j.jaap.2018.05.005>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Diffusion of CO₂ and Fractional Free Volume in Crystalline and Amorphous Cellulose

Abdul Salam Mohammad¹, Joseph J. Biernacki¹, Scott. Northrup² and Michael Adenson¹

¹Department of Chemical Engineering, Tennessee Tech University, Cookeville, TN 38505

²Department of Chemistry, Tennessee Tech University, Cookeville, TN 38505

Highlights

- Diffusion of CO₂ in cellulose was estimated using molecular dynamic simulation
- Diffusion of CO₂ progresses by a jumping mechanism
- Estimated diffusivities compare favorably with comparable experimental results
- A Thiele Modulus analysis shows CO₂ diffusion is relevant at pyrolysis conditions

Abstract

Molecular-scale modeling was used to estimate the diffusion coefficient for CO₂ in crystalline and amorphous cellulose. Using the molecular mechanics force field, PCFF, molecular dynamics simulations were performed on CO₂-cellulose systems at temperatures between 300 and 800 K using an NPT ensemble. The mean-square displacement for CO₂ molecules at each time step was measured, and the diffusivity of CO₂ in cellulose calculated. For temperatures between 300 and 800 K, the diffusivity of CO₂ through crystalline cellulose was estimated to be between 3.33×10^{-9} and $3.20 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$, and between 2.33×10^{-8} and $9.44 \times 10^{-6} \text{ cm}^2 \text{ s}^{-1}$ for amorphous cellulose. The effect of temperature on the diffusivity of CO₂ is small with an activation energy of between 16.5 and 16.9 kJ/mol for crystalline cellulose and between 10.2 and 15.1 for amorphous cellulose.

Download English Version:

<https://daneshyari.com/en/article/8954824>

Download Persian Version:

<https://daneshyari.com/article/8954824>

[Daneshyari.com](https://daneshyari.com)