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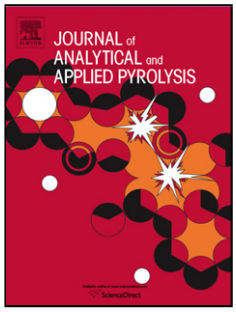

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Authors: Abdul Salam Mohammad, Joseph J. Biernacki, Scott. Northrup, Michael Adenson

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Diffusion of CO_2 and Fractional Free Volume in Crystalline and Amorphous Cellulose

Abdul Salam Mohammad[1], Joseph J. Biernacki[1], Scott. Northrup[2] and Michael Adenson[1]

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

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

Highlights

- Diffusion of CO_2 in cellulose was estimated using molecular dynamic simulation
- Diffusion of CO_2 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 CO_2 in crystalline and amorphous cellulose. Using the molecular mechanics force field, PCFF, molecular dynamics simulations were performed on CO_2-cellulose systems at temperatures between 300 and 800 K using an NPT ensemble. The mean-square displacement for CO_2 molecules at each time step was measured, and the diffusivity of CO_2 in cellulose calculated. For temperatures between 300 and 800 K, the diffusivity of CO_2 through crystalline cellulose was estimated to be between 3.33×10^{-9} and 3.20×10^{-6} $cm^2\ s^{-1}$, and between 2.33×10^{-8} and 9.44×10^{-6} $cm^2\ s^{-1}$ for amorphous cellulose. The effect of temperature on the diffusivity of CO_2 is small with an activation energy of between 16.5and 16.9 kJ/mol for crystalline cellulose and between 10.2 and 15.1 for amorphous cellulose.