Transport of Pyrolysis Fragments in Cellulose – A Molecular Dynamics Study

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Pyrolysis of lingocellulosic biomass could become a significant source of renewable chemicals and fuels in the near future. In addition to bio-oil production, fast pyrolysis of biomass produces significant quantities of permanent gases, including H_2, CO, CO_2, and CH_4, also known as synthesis gases. Heating of wood, grass and other cellulose rich plants matter in the absence of air also produces chemical fragments that resemble the lingocellulosic starting materials. The processes that control these events are complex and not yet well understood. Among the many questions is the rate at which the bio-pyrolysis fragments are transported through the lingocellulosic frame work. The purpose of this study was to use molecular modeling to simulate the transport of pyrolysis product fragments through a model cellulose structure. Materials Studio was used to create and optimize a model for crystalline cellulose. To simulate the diffusion of product gases, a molecule of CO_2 was placed within the cellulose matrix as a simple test bed. Using the FORCITE module and the molecular mechanics force field, pcff, molecular dynamics was performed on the CO_2-cellulose system at 598 K with an NPT ensemble. The mean-square displacement at each time step was measured and the diffusivity of CO_2 calculated. At 598 K, the diffusivity of CO_2 through cellulose was calculated to be 0.4403×10^{-12} cm^2 s^{-1}. It appears that the effect of temperature on the diffusivity of CO_2 is small. At 298K, the diffusivity of CO_2 through crystalline cellulose was found to be 0.1720×10^{-12} cm^2 s^{-1}.