

Multiscale molecular approach to model bioenergy with carbon capture and storage processes

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Bioenergy with Carbon Capture and Storage (BECCS) combines biomass energy production with carbon capture and storage. In particular, a large amount of pure CO₂ is produced in sugarcane-based ethanol production. A more sustainable and long-term carbon capture and storage alternative can be found on geological sites near Ethanol production plants in Brazil. Here, we propose and apply a multiscale computational framework that will enable the study of the mechanisms of CO₂ mineralisation reactions and obtain essential parameters for reservoir-scale models. Multiscale molecular simulations were used to determine the fluid-rock interface properties, the diffusivity of CO₂, mineralisation reactions, phase change, and modifications in the mechanical/structural properties of the geological components over time due to changes in porosity and permeability. The methods range from first principles calculations of molecular dynamics and lattice Boltzmann methods to modelling the CO₂ mineralisation reactions on atomic and pore scales. These implemented methodologies and findings can lead to process optimisation for CO₂ storage in the subsurface, coupling nano to macro scales with reservoir simulation tools and modelling and selecting the optimal reservoir conditions for the mineralisation of CO₂ from biofuels production.

