BITS Pilani
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Department of Chemical Engineering

Book of Abstracts

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Nanotechnology For:

- ➔ Waste to Wealth
- ➔ Pollution abatement
- ➔ Renewable Energy
- ➔ Advanced Materials
- ➔ Sensors and Flexible Electronics
- ➔ Biomedical Applications
- ➔ Nanofluid Applications

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NANOTECHNOLOGY FOR RENEWABLE ENERGY

1D). A structural device is modeled for optimizing absorber layer thickness, and thus the solar cell efficiency, using various non-toxic buffer layers like CdS, ZnO, In_2S_3, ZnS, and ZnSe with the thickness of 40 nm. The modeled structure with the optimized thickness (0.2µm-2.5µm) resulted in higher efficiency (~22%) Antimony Chalcogenide thin-film Solar Cells. The modeled heterojunction Solar Cell is more inexpensive than the readily available materials.

Simulation of fixed bed adsorption for Biogas Upgrading

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Heroic efforts have been devoted to developing clean sources of energy that can contribute to keeping global warming below 2ºC in the coming 30 years. Biogas is a renewable source of energy that can be easily produced by the treatment of agricultural, municipal, and industrial wastes. Furthermore, biogas can be a decentralized alternative to produce clean energy in Portugal and India, as both have a large quantity of feedstock. The second main component of biogas is CO_2, which decreases its heating value by half relative to natural gas. Therefore, biogas needs to be upgraded (by removing CO_2) to obtain biomethane that can be either injected into natural gas networks or directly used as a vehicle fuel. In this way, adsorption processes are a promising alternative to biogas upgrading as it presents a lower energy cost, is easy to operate, can provide higher purity and recovery, as compared to other methods, and especially for the possibility of regenerating the adsorbent material without generating by-products. In this view, this work seeks to develop an adsorption simulator to study the separation of $CO_2/CH_4/N_2$ mixtures in a fixed bed. To achieve this objective, a mathematical model has been developed to describe the adsorption of mixtures in a fixed bed solved through numerical methods available in the literature. The adsorption mathematical model, derived from mass and energy conservation laws, was implemented in a personal computer to predict the dynamic behavior of the adsorption process. Moreover, this mathematical model includes both effects of axial dispersion and mass-transfer resistances considering an overall effective rate mass-transfer (KLDF) from the linear driving force model. The numerical implementation was performed in the MATLAB simulation environment. To solve the mathematical model the method of lines was used, being the spatial coordinates discretized by orthogonal collocation, and the resulting ordinary and algebraic differential equations were solved with a stiff integrator, ode15s, available in the MATLAB library. The implemented model was evaluated and validated by simulating experimental data of fixed-bed adsorption of CO_2, CH_4, and N_2 on binder-free zeolite 4A and KY performed in our laboratory. In summary, the simulator implemented in this work is a versatile tool to describe the adsorption process and is useful in process simulation.