What is DAC?

- The Direct Air Capture model that we are going to use is based on a packed bed reactor model, where there is a column with several beds embedded with amine-functionalized solid sorbents.

- A sorbent is a basic substance that allows the acidic CO_2 to be adsorbed, ie. holds CO_2 molecules on its surface via adhesion.

- This model focuses on passing ambient air into the reaction column, where CO_2 is adsorbed onto the surface of the sorbent.

What is DAC?

- Then the CO_2 is extracted by either a temperature or a vacuum swing.

- Other air particles such as excess O_2 are removed, steam is fed to the reactor, and the CO_2 undergoes desorption through the temperature swing. The vacuum swing then is used to cool the reactor and extract the water.

- For our simulation model, we will be studying the packed bed reactor by discretizing the column length into equal parts and simultaneously calculating the parameters of concern in each section to get the results of the model.

Where it is used? Why important?

- Direct Air Capture (DAC) is often used on an industrial scale in order to reduce the impact of CO_2 emissions in hopes of fighting global warming.

- It is possible to acquire a zero net carbon dioxide emissions with DAC, and the extracted carbon dioxide can be reallocated to create synthetic fuels or in the processing of foods, and materials that are consumed on a daily basis

- The future of energy consumption and CO_2 will be greatly affected by DAC, as the development of direct air capture technologies continue to advance in hopes of producing zero or negative net carbon dioxide emissions.

What do we aim to achieve?

- To successfully simulate a digital model of Direct CO2 Capture system using Python in order to introduce chemical engineering students to concepts relating to rate of reaction, mass balance, and energy balance used in the DAC models

- To introduce and create a visual model of the mechanism that is easy for students to understand.

- Compare and evaluate the changes in the model based on various set parameters and how they apply to the real world.

Assumptions

- For our model, we have made the following assumptions:
  - The velocity of the air is constant throughout the column
  - The temperature of the reactor walls are the same throughout the column
  - No axial diffusion of mass or conduction of heat
  - No radial concentration or temperature gradients
  - The air that is passed through the column is dry air so minimal humidity in the air.

General Formulas

- Rate of Reaction

$$r_{CO2} = [k_T\,(P_{CO2}\left(1 - \left(\frac{q}{q_s}\right)^{t_h}\right)^{\frac{1}{t_h}} - \frac{q}{bq_s})]$$

- Mass Balance

$$\varepsilon_r \frac{\partial C_{CO2}}{\partial t} = \; - v\left(\frac{C_{CO2_1} - C_{CO2_0}}{\Delta z}\right) - r_{CO2}(1 - \varepsilon_r)\rho_s$$

- Energy Balance

$$\left[(1 - \varepsilon_r)\rho_s C_{p_s} + \varepsilon_r \rho_g C_{p_g}\right]\frac{\partial T}{\partial t} = \left(\frac{\partial}{\partial z}\left(- v_0 \rho_g C_{p_g} T\right)\right) + ((1 - \varepsilon_r)\,\rho_s\left(\Delta H_{CO2}\, r_{CO2}\right)) + a_s h\,(T_w - T)$$

User Input

- Volume of the reactor bed
- Initial CO_2 concentration
- Initial temperature
- Volumetric flow rate of CO_2 passed
- ε (Porosity of the bed)
- Material of the Wall

Changing Parameters that are calculated by the model

- Rate of reaction
- Rate of adsorption of CO_2
- Temperature
- Concentration of CO_2 in the passed air

Questions

- What values of the changing parameters together would give the most efficient result (ie, most CO_2 adsorption in minimal temperature change)?
- How does changing the value of ΔH (change in enthalpy) or ε (porosity of the bed) affect the adsorption and desorption of CO_2?
- What operational variables would be affected if we used humid air instead of dry air on this DAC model? How would this change affect each of our changing parameters?
- Look up some relevant properties of KOH. How would changing sorbents affect the calculations of our model?