

Sizing a Catalytic PBR: From Kinetic Mechanism to Transport Considerations,
to Macroscale Mixing Model.

n-Butane is to be isomerized to iso-butane, as part of an overall industrial plant process. You are charged with designing the catalytic packed-bed reactor for converting 95% of the n-butane to iso-butane. You have an unlimited supply of ZSM-5 catalyst, which is an acidic clay zeolite catalyst with good activity for this reaction.

A. **Explain the kinetic data.** The Research Department has provided you with the following information, culled from several accurate and verified kinetic experiments:



- First-Order w.r.t. Catalyst Weight (in absence of transport limitations)
- First-Order w.r.t. N-Butane Partial Pressure (in absence of transport limitations)
- Zero-Order w.r.t. Iso-Butane Partial Pressure (in absence of transport limitations) at low partial pressures, First-Order w.r.t. Iso-Butane Partial Pressure at high partial pressures.

$$R_A = - (1.5 \times 10^{-1} \text{ mol.g-cat}^{-1} \cdot \text{L}^{-1}) \cdot C_A \cdot W_{\text{ZSM-5}} [=] \text{ mol.L}^{-1} \cdot \text{sec}^{-1} @ 350^\circ\text{C}.$$

If the mechanism for this reaction is a two-step mechanism:



Which step is the rate-limiting step (or are both steps at equal rates?) to produce this kinetics?

B. **Size the Catalyst.** For a first-order reaction, the maximum catalyst effectiveness is 100% ($\eta = 1.0$). Realistically, an effectiveness of 95% ($\eta = 0.95$) represents a good balance between catalyst size and reactor size. If both butane isomers have an effective diffusivity in ZSM-5 of $1 \times 10^{-6} \text{ m}^2 \cdot \text{s}^{-1}$, and there are NO EXTERNAL DIFFUSION LIMITATIONS, what size catalyst spheres are needed to obtain an effectiveness of 0.95? Assume, for simplicity, that $K_B \ll 1$.

C. **Size the Reactor.** Calculate the total amount of catalyst required for this PBR to achieve an outlet conversion of 99%. Neglect pressure-drop, and assume that the effectiveness factor is constant throughout the bed. The N-Butane feed is 5 mol/s @ 10 bar & 350°C. Assume that a cooling jacket maintains constant operating temperature throughout. Assume, for simplicity, that $K_B \ll 1$.