ChE445_Chemical Reactor Analysis II_Seminar11_Winter2020

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1 Seminar 11. Evaluation of internal MTL and conversion in a PBR.

Q1. Evaluation of internal MTL and conversion in a PBR.

Nitrous oxide (N_2O) has a greenhouse gas global warming potential that is almost 300 times higher than that of carbon dioxide. Its catalytic reduction to harmless N_2 can be done using CH_4, NH_3 or H_2.

Consider gas-phase constant-density N_2O hydrogenation on a Pt/SiO_2 catalyst that follows an intrinsic first order to N_2O and apparent 0 to hydrogen due its large excess. There are no external transfer limitations, assume negligible pressure drop. The catalyst pellet can be considered isothermal. Evaluate internal mass transfer limitations: $P = 102000\ pa$, Pore diameter in individual catalyst particle, $3 * 10^{-9} m$, Particle porosity= 0.2, Tortuosity in a particle= 4, Intrinsic rate constant (based on N_2O), $1.7 \frac{m^3\ fluid}{(kg\ cat*s)}$ at 573 K, Catalyst density, $4000 kg/m^3$, Reaction activation energy, $120000 J/mol$, Volumetric velocity at STP ($0\ ^oC$, $100000\ Pa$), $0.8\ m^3/s$, Catalyst mass in PBR, $2kg$

a). Assess the particle size effect: For catalyst particle diameters = $(3, 6, 12, 24, 48, 96, 192, 384)$ μm calculate molecular diffusivity, Knudsen diffusivity of N_2O, pore diffusivity of N_2O, effective diffusivity of N_2O, intrinsic rate constant $[\frac{m^3_{fl}}{m^3_{cat}*s}]$, Thiele modulus, Internal effectiveness factor, Volumetric velosity at reaction conditions, $[m^3_{fl}/s]$, conversion and ideal PBR conversion,%.

write down formulas you used and show the units conversion, when necessary. Sketch a graph "X vs. particle size" for an ideal and real PBR and clearly mark final and initial points. On this graph, circle a part of the real PBR curve where there are no MTL ("kinetic regime").

Remember that internal effectiveness factor is just a coefficient in front of the intrinsic rate law based on external surface concentration.

b). Assess the temperature effect: For different temperatures $[457, 493, 533, 573, 613, 653, 693, 733]$ and catalyst particle diameters of 48 μm calculate molecular diffusivity, Knudsen diffusivity of N_2O, pore diffusivity of N_2O, effective diffusivity of N_2O, intrinsic rate constant $[\frac{m^3_{fl}}{m^3_{cat}*s}]$ and Intrinsic rate constant, $[\frac{m^3_{fl}}{m^3_{cat}*s}]$, Thiele modulus, Internal effectiveness factor, Volumetric velosity at reaction conditions, $[\frac{m^3_{fl}}{s}]$, conversion and ideal PBR conversion,%.

Write down (an) additional formula(s) you used. Sketch a final "X vs. T" for an ideal and real PBR and clearly mark final and initial points. On this graph, circle a part of the real PBR curve where there are no MTL ("kinetic regime").

At what temperatures (lower or higher) the internal MTL become more significant and why?