ChE445_Chemical Reactor Analysis II_Seminar12_Winter2020_Solution

April 7, 2020

Q1. Internal, external and global mass transfer limitations at isothermal conditions. Review of TOF.

(Fogler Ed5. Chp 15 & Hayes Ch 5)

A reaction rate was measured in a PBR without pressure drop at the following isothermal conditions:

Run#	Particle radius, mm	Total flow rate,mol/s	Observed rate,$mol/(g_{cat}.h)$
1	0.1	600	0.50
2	0.2	400	0.50
3	0.2	800	0.49
4	0.2	1200	0.51
5	0.4	400	0.26
6	0.4	800	0.24
7	0.4	1200	0.25
8	4	400	0.02
9	4	800	0.05
10	4	1200	0.05

Hint: remember that these are experimental data subject to an experimental error.

a). What are the internal, external and global effectiveness factors for runs 1-4? Explain your choices and provide relevant calculations, where necessary.

b). What are the internal, external and global effectiveness factors for runs 5-7? Explain your choices and provide relevant calculations, where necessary.

c). What are the internal, external and global effectiveness factors for runs 9-10? Explain your choices and provide relevant calculations, where necessary.

d). What are the internal, external and global effectiveness factors for run 8? Explain your choices and provide relevant calculations, where necessary.

e). Calculate TOF if the catalyst contains $5wt.\%$ Pd of 30% dispersion. Pd molar mass is $106g/mol$.

(Hint: TOF is characteristic of an active site, it reflects intrinsic catalyst activity and must calculated based on the intrinsic rate law).

Answer to Q1

a.) For runs 1-4, variables are particle radius, R_p and total flow rate, F_T.

but observed rate is alomost the same $0.50 \pm 0.01\ \frac{mol}{gr}$ so this is an intrinsic kinetic regime, $\Omega = \eta_{ext} = \eta_{int} = 1$

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b.) For runs 5-7 the total flow rate, F_T, does not have an effect on the reaction rate, so there are no external MTL ($\eta_{ext} = 1$)

but the observed rate= $0.25 < 0.50$ in kinetic regime (for runs 1-4) , so there are internal MTL.

$\eta_{int} = \frac{Observed\ rate\ without\ external\ MTL}{Intrinsic\ rate} = \frac{0.25}{0.5} = 0.5$

$$\Omega = Overall\ \ effectiveness\ \ factor$$

$$\Omega = \frac{Actual/observed\ overal\ rate\ of\ reaction}{Rate\ that\ would\ result\ if\ the\ entire\ surface\ were\ exposed\ to\ the\ bulk\ condition,\ C_{Ab}, T_b} \quad (1)$$

$$\Omega = \eta_{int} * \eta_{ext} = 0.5 * 1 = 0.5 \quad (2)$$

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c.) For runs 9-10, the total flow rate, F_T, does not have an effect on the reaction rate, so there are no external MTL $\eta_{ext} = 1$.

$\eta_{int} = \frac{Observed\ rate\ without\ external\ MTL}{Intrinsic\ rate} = \frac{0.05}{0.50} = 0.1$

$\Omega = \eta_{int} * \eta_{ext} = \eta_{int} * 1 = 0.1$

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d.) For run 8: Where both external and internal limitation affect the rate.

From runs 9 and 10 for $R_{particle} = 4mm$, $\eta_{int} = 0.1$

$$\Omega = \frac{observed\ rate}{Intrinsic\ rate} = \frac{0.02[run8]}{0.50[run\ 1-4]} = 0.04 \quad (3)$$

$$\Omega = \eta_{int} * \eta_{ext} \quad (4)$$

$$\eta_{ext} = \frac{0.04}{0.1} = 0.4 \quad (5)$$

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e.) TOF (turn over frequency) is intrinsic reaction rate as $[\frac{mol_A}{mol_{Active\ sites} * s}]$.

Use runs $1-4$, rate 0.5 to calculate TOF as follows:

$$TOF[\frac{mol_A}{mol_{active\ site} * s}] = 0.5\frac{mol}{g_{cat} * h} * \frac{1}{0.05}\frac{g_{cat}}{g_{pd}} * 106\frac{g_{Pd}}{mol_{Pd}} * \frac{1}{0.3}\frac{mol\ Pd}{mol\ surf(active\ site)\ Pd} * \frac{1}{3600}\frac{h}{s} = 0.98s^{-1} \quad (6)$$

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